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Electronic Supplementary Information

Mesoporous Stilbene-based Lanthanide Metal Organic Frameworks: Synthesis, Photoluminescence and Radioluminescence Characteristics

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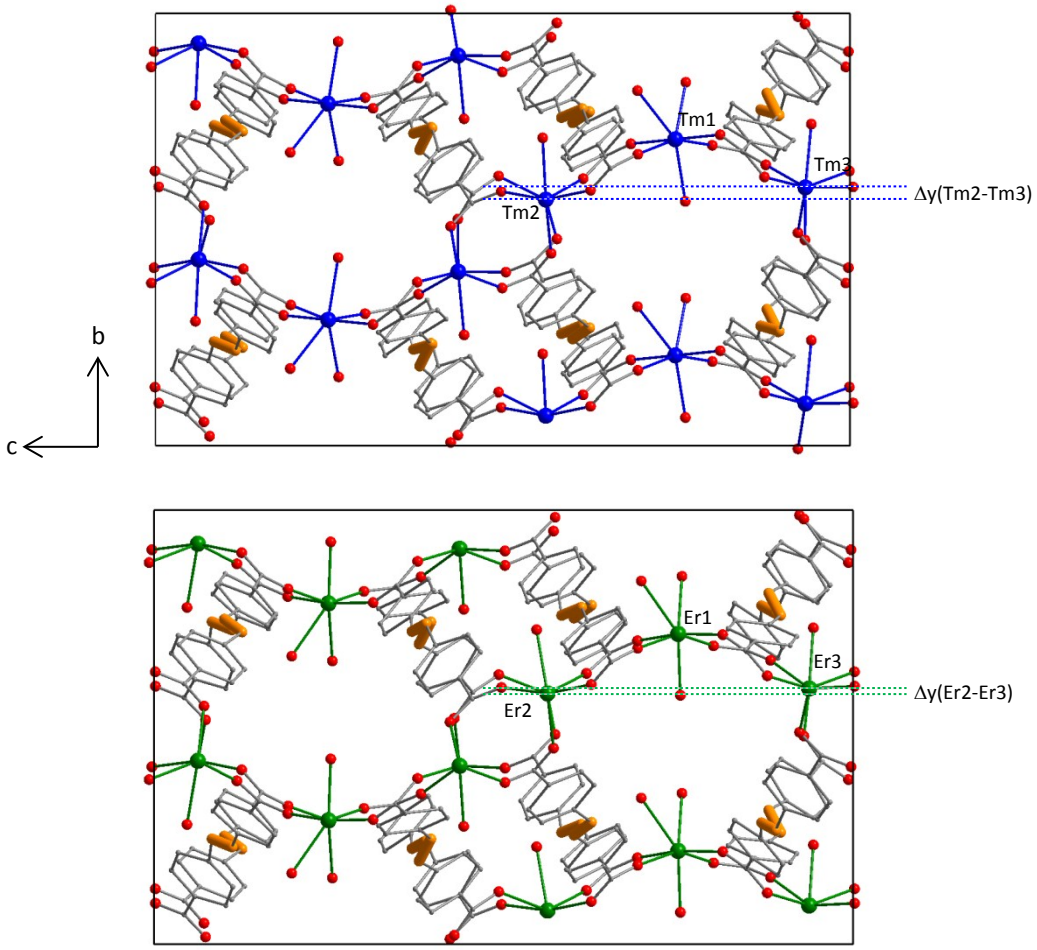
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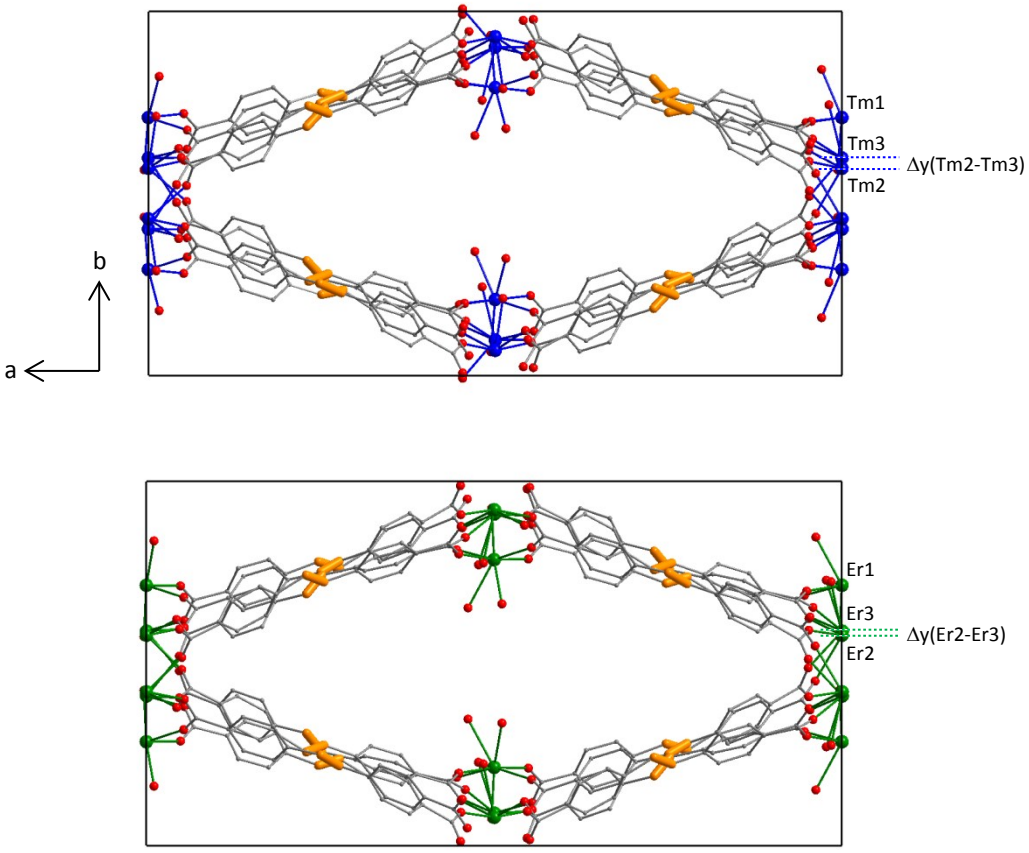
Tm2
Δy(Tm2-Tm3)
b
c
Er1
Er3
Er2
Δy(Er2-Er3)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Er1
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Er2

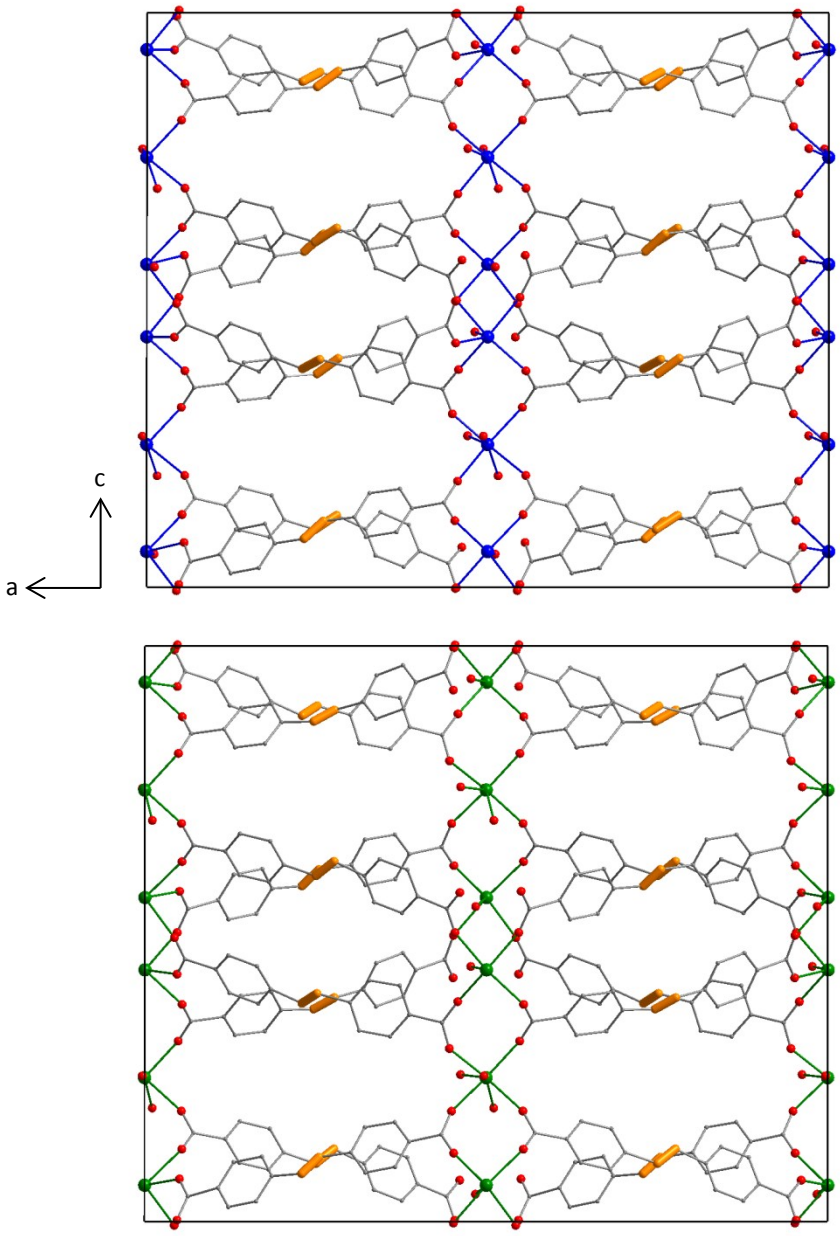

Figure S1: Unit cells of Tm (top) and Er structures (bottom) as refined in Cc. The structures are viewed along unit cell vectors a, b and c, respectively. Relative displacement Δy of M2 and M3 are highlighted. Central olefin groups are also highlighted in order to illustrate orientation of stilbene ligands.

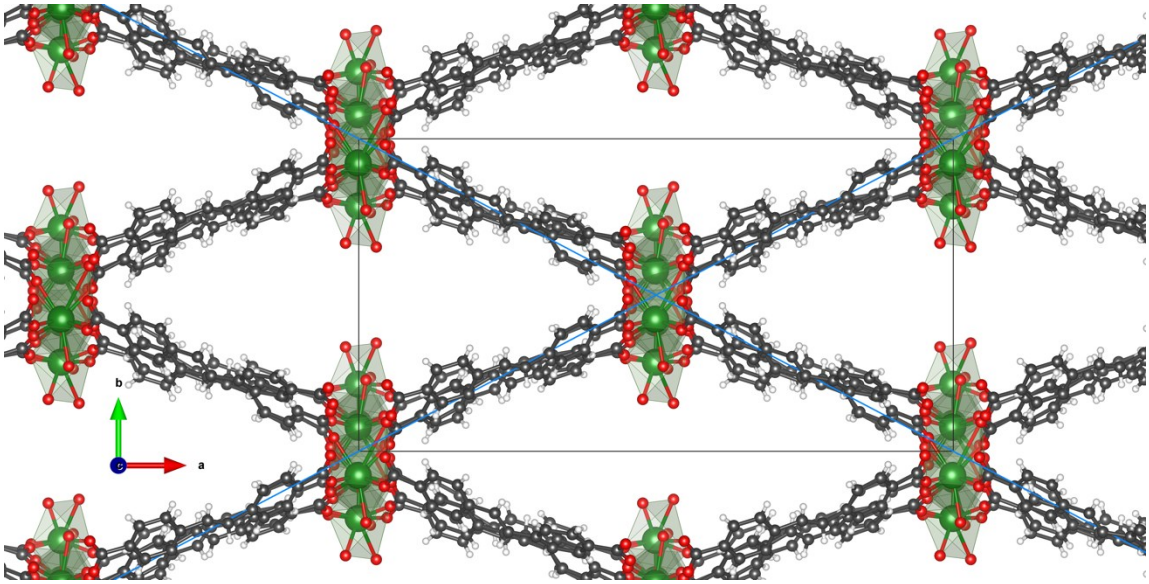

Figure S2. View of the ligand-metal interconnectivity along the channel [001] direction for **1**. Hydrogen atoms and solvent molecules are omitted for clarity.

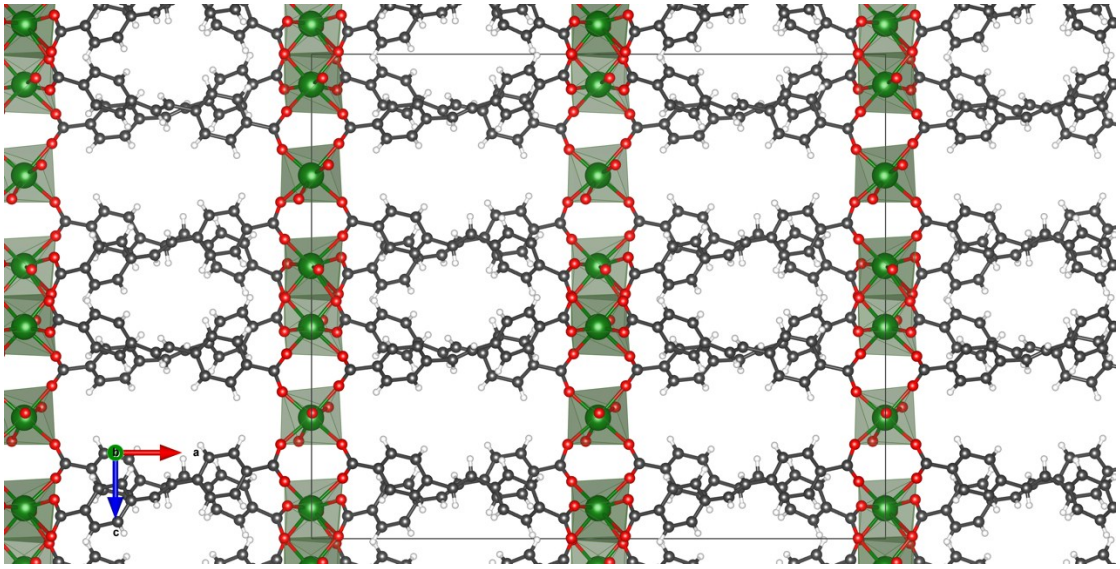

Figure S3. Viewing the ligand-metal interconnectivity perpendicular to the channel direction (along the [010] axis) shows the series of diagonal bracing of stilbene linkers between the coordination chains. Hydrogen atoms and solvent molecules are omitted for clarity.

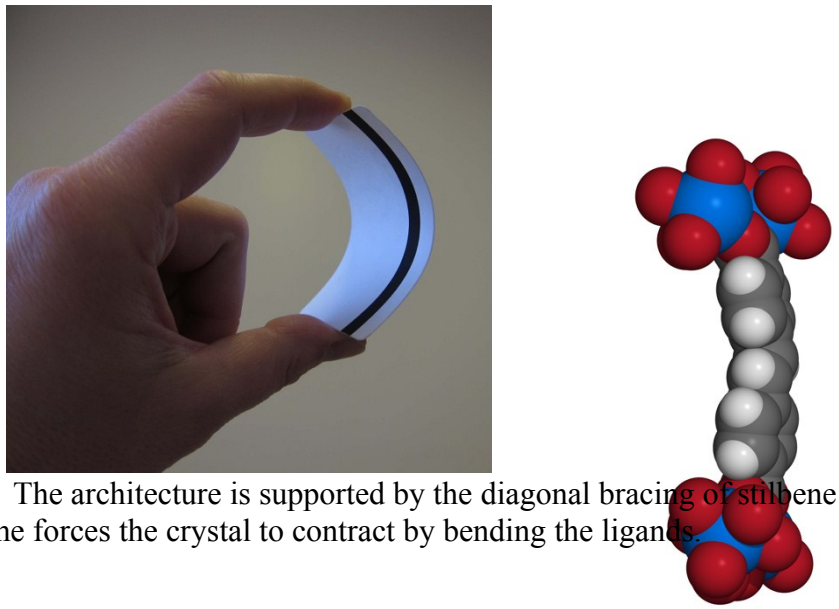

Figure S4. The architecture is supported by the diagonal bracing of stilbene linkers but the large pore volume forces the crystal to contract by bending the ligands.

There are strong electron density peaks within 1.0 Å to the lanthanide atoms. There are strong peaks located around 3.4 Å from the lanthanide atoms that are subtended by the stilbene ligands in the planes parallel to the *bc*-plane. Although these peaks are located towards the interior of the channels it was not possible to locate the remainder of the DEF molecule, even as a rigid group. The blurred electron density along this plane is thought to be due to unresolved twinning. Some disorder is expected in such an open structure with such a large pore volume. The large pore volume forces the crystal to contract by bending the ligands (like bending a long and flat object by compressing it at either ends, Figure S4). Perhaps it is this strain that causes the lanthanide atom units of parallel strains to buckle along *c*-direction (with breaking of symmetry and large residual densities). This shift of lanthanide units may further contribute to the contraction.

Table S1. Comparison of R-values of the refinement of squeezed structures with equivalent settings

		Er	Tm
Cmcm	R1	0.1108	0.1786
	Δx(M2-M3)	0	0
	Δy(M2-M3)	0	0
	Δz(M2-M3)	0	0
	Z' (stilbene)	1	1
$Cmc2_1$	R1	0.0748	0.0704
	Δx(M2-M3)	0	0
	Δy(M2-M3)	0.195	0.445
	Δz(M2-M3)	0.004	0.029
	Z' (stilbene)	2	2
C2cm (Ama2)	R1	0.0811	0.1268
	Δx(M2-M3)	0	0
	Δy(M2-M3)	0	0
	Δz(M2-M3)	0	0
	Z' (stilbene)	2	2
C2/c	R1	0.0956	0.1446
	Δx(M2-M3)	0.007	0.007
	Δy(M2-M3)	0	0
	Δz(M2-M3)	0	0
	Z' (stilbene)	2	2
Cc	R1	0.0720	0.0687
	Δx(M2-M3)	0.006	0.001
	Δy(M2-M3)	0.184	0.451
	Δz(M2-M3)	0.008	0.057
	Z' (stilbene)	4	4

Frameworks of both compounds are isostructural and refine as severely disordered models in Cmcm. $Cmc2_1$, C2cm (Ama2) and C2/c are non-isomorphic subgroups of Cmcm that retain the C-centred lattice and the c-glide plane. Cc is a subgroup of all three, again under retention of the lattice and the glide plane.

Table S1 compares R-values of the refinement of squeezed structures with equivalent settings (anisotropic metal atoms, isotropic C and O atoms, H atoms fixed to parents C atoms (AFIX43 , U_{iso} 1.2 times of that parent C) ; stilbene ligands were treated with equivalent SAME and SIMU restraints). Cc and C2/c were refined as pseudo-merohedral twins.

Metal atoms M2 and M3 show slightly different y-positions (which is slightly more pronounced in the case of Tm); these are only resolved in $Cmc2_1$ and Cc as these spacegroups do not impose

symmetry constraints on the y-parameters of both atoms. The refinement in these two spacegroups gave the best agreement values.

Z' (stilbene) gives the number of crystallographically unique stilbene ligands.

ErSDC (SDC = stilbene dicarboxylate)

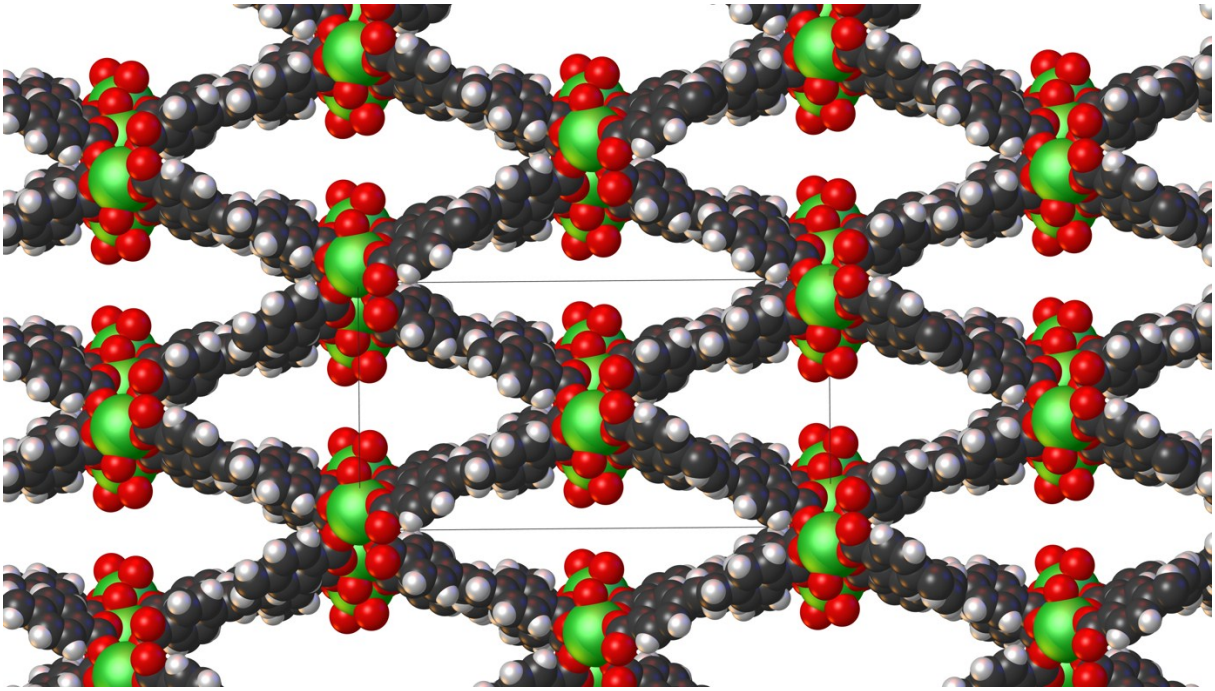

Table S2 Crystal data and structure refinement for ErSDC.

Identification code	ErSDC
Empirical formula	$C_{64}H_{40}Er_3O_{21}$
Formula weight	1646.74
Temperature/K	100(2)
Crystal system	monoclinic
Space group	Cc
a/Å	30.6336(8)

b/Å	16.0923(6)
c/Å	25.8791(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	12757.4(8)
Z	4
ρ_{calc}g/cm^3	0.857
μ/mm^{-1}	1.992
F(000)	3184.0
Crystal size/mm^3	0.244 × 0.24 × 0.19
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.09 to 50.054
Index ranges	-33 ≤ h ≤ 36, -16 ≤ k ≤ 19, -30 ≤ l ≤ 30
Reflections collected	36038
Independent reflections	18590 [R_{int} = 0.0489, R_{sigma} = 0.0691]
Data/restraints/parameters	18590/2131/784
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0803, wR_2 = 0.2066
Final R indexes [all data]	R_1 = 0.1134, wR_2 = 0.2307
Largest diff. peak/hole / e Å^{-3}	2.75/-1.01
Flack parameter	?

Table S3. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for ErSDC. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*y*	*z*	U(eq)
Er1	4994.5(10)	5892.3(7)	628.1(12)	52.4(4)
Er2	4991.0(11)	7149.7(7)	2502.9(14)	74.1(3)
Er3	4990(1)	5775.8(7)	4371.8(12)	49.0(3)
O1	5194(10)	7357(19)	491(11)	160(9)
O2	5012(7)	5733(10)	2407(7)	90(6)
O3	5294(8)	8461(14)	2284(10)	252(17)
O4	4777(8)	8339(15)	2990(9)	252(17)
O5	5122(11)	7277(18)	4446(11)	160(9)
O11	4489(7)	7032(9)	1967(7)	93(5)
O12	4564(7)	6512(9)	1185(7)	92(5)
C11	4346(6)	6834(5)	1536(6)	92(4)
C12	3867(6)	6988(8)	1409(8)	96(4)
C13	3591(7)	7344(12)	1765(9)	100(5)
C14	3144(8)	7479(14)	1637(10)	102(5)
C15	2983(7)	7266(13)	1166(10)	103(5)
C16	3261(7)	6916(13)	819(10)	101(5)
C17	3710(7)	6767(12)	930(9)	99(5)
C18	2516(8)	7420(17)	1045(14)	106(5)
O21	5476(6)	7125(9)	1844(5)	67(4)
O22	5545(6)	6142(8)	1235(5)	62(4)
C21	5675(4)	6719(6)	1512(3)	63(3)

C22	6150(5)	6973(9)	1441(6)	66(3)
C23	6309(6)	7614(11)	1740(7)	68(4)
C24	6752(6)	7872(12)	1686(8)	71(4)
C25	7001(6)	7466(11)	1331(7)	73(4)
C26	6848(6)	6836(12)	1032(8)	71(4)
C27	6406(6)	6570(11)	1084(7)	67(4)
C28	7456(6)	7781(16)	1304(10)	76(4)
O31	5443(7)	4810(10)	740(7)	115(6)
O32	5428(7)	3877(12)	98(6)	116(6)
C31	5590(4)	4229(7)	478(4)	114(5)
C32	6033(5)	3880(12)	634(8)	119(5)
C33	6247(8)	4222(16)	1050(10)	123(6)
C34	6663(8)	3925(17)	1215(11)	125(6)
C35	6856(8)	3289(16)	956(11)	126(6)
C36	6644(8)	2953(17)	545(11)	124(6)
C37	6228(8)	3237(15)	371(10)	122(6)
C38	7289(9)	3020(20)	1156(14)	127(7)
O41	5466(7)	5933(10)	-52(5)	81(5)
O42	5517(6)	5217(9)	-808(6)	87(5)
C41	5631(4)	5715(6)	-468(4)	85(4)
C42	6060(4)	6150(10)	-589(8)	94(4)
C43	6221(7)	6720(12)	-242(9)	98(5)
C44	6624(7)	7130(14)	-349(9)	100(5)
C45	6854(7)	6972(14)	-788(9)	101(5)

C46	6694(7)	6409(14)	-1130(9)	101(5)
C47	6291(7)	5989(13)	-1035(9)	100(5)
C48	7269(7)	7437(17)	-857(12)	102(5)
O51	5529(5)	6755(9)	3054(5)	64(4)
O52	5542(6)	5992(8)	3751(6)	56(4)
C51	5711(4)	6492(6)	3448(4)	57(3)
C52	6168(4)	6821(8)	3551(6)	57(3)
C53	6387(6)	7377(11)	3241(7)	62(4)
C54	6817(6)	7654(12)	3364(8)	64(4)
C55	7012(6)	7358(11)	3798(7)	67(4)
C56	6798(5)	6809(11)	4106(8)	65(4)
C57	6368(5)	6524(10)	3989(7)	60(4)
C58	7458(6)	7616(15)	3956(10)	71(5)
O61	4464(8)	6914(10)	3055(7)	109(6)
O62	4533(7)	6301(9)	3821(7)	100(6)
C61	4334(5)	6701(6)	3487(6)	102(5)
C62	3870(5)	6977(9)	3610(9)	102(5)
C63	3649(7)	7424(13)	3240(10)	105(6)
C64	3213(7)	7705(15)	3325(11)	106(6)
C65	3014(7)	7529(15)	3781(10)	109(6)
C66	3234(8)	7088(15)	4146(11)	107(6)
C67	3670(7)	6797(13)	4073(10)	103(6)
C68	2561(8)	7821(19)	3875(13)	113(7)
O71	4582(5)	4568(8)	4323(6)	65(4)

O72	4525(5)	3718(9)	4990(5)	59(4)
C71	4396(4)	4022(6)	4578(4)	61(3)
C72	3968(4)	3706(9)	4354(6)	64(4)
C73	3827(6)	4046(11)	3895(7)	71(4)
C74	3425(6)	3745(12)	3689(8)	76(4)
C75	3198(6)	3145(12)	3943(8)	77(4)
C76	3343(6)	2814(12)	4394(8)	76(4)
C77	3744(5)	3097(11)	4614(8)	70(4)
C78	2782(6)	2857(15)	3710(10)	79(5)
O81	4540(6)	5977(11)	5025(5)	85(5)
O82	4526(6)	5135(9)	5723(7)	90(5)
C81	4393(4)	5696(7)	5436(4)	87(5)
C82	3974(4)	6114(11)	5620(8)	90(5)
C83	3798(6)	6746(13)	5330(9)	95(5)
C84	3406(7)	7119(15)	5516(10)	99(5)
C85	3208(7)	6869(15)	5959(10)	102(5)
C86	3387(7)	6244(15)	6241(10)	99(5)
C87	3780(7)	5853(14)	6071(9)	95(5)
C88	2801(7)	7306(19)	6112(13)	108(6)

Table S4. Anisotropic Displacement Parameters ($Å^2×10^3$) for ErSDC. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Er1	25.7(7)	68.8(7)	62.6(8)	13.0(6)	-1.5(10)	12.4(9)
Er2	33.2(5)	116.5(9)	72.8(6)	-1.6(10)	-1.4(10)	-4.9(15)
Er3	19.8(6)	67.5(7)	59.7(8)	-14.2(6)	-2.2(9)	-5.6(9)
O1	173(13)	142(11)	166(11)	29(10)	-5(10)	-23(9)
O2	62(9)	110(10)	99(12)	34(9)	9(12)	3(12)
O3	253(18)	246(18)	256(18)	-3(9)	21(8)	-2(9)
O4	253(18)	246(18)	256(18)	-3(9)	21(8)	-2(9)
O5	173(13)	142(11)	166(11)	29(10)	-5(10)	-23(9)
O11	83(7)	104(8)	94(6)	-10(5)	-6(5)	18(6)
O12	81(6)	104(8)	92(6)	-10(6)	-7(5)	18(6)
C11	83(6)	99(6)	92(6)	-8(4)	-4(4)	15(4)
C12	82(6)	110(7)	96(7)	-11(6)	-5(5)	19(5)
C13	84(6)	116(9)	99(7)	-14(6)	-4(5)	20(6)
C14	84(6)	120(9)	103(8)	-17(7)	-5(5)	22(6)
C15	85(6)	121(9)	104(8)	-18(7)	-6(5)	23(6)
C16	84(6)	118(9)	102(7)	-16(7)	-8(5)	23(6)
C17	84(6)	115(9)	98(7)	-13(6)	-7(5)	22(6)
C18	85(7)	125(11)	108(9)	-20(9)	-7(6)	25(6)
O21	59(6)	73(6)	70(6)	-2(5)	8(5)	-21(5)
O22	53(6)	69(6)	64(6)	3(5)	6(5)	-19(5)

C21	56(5)	68(5)	64(5)	3(4)	5(4)	-18(4)
C22	56(5)	74(6)	67(6)	4(5)	5(4)	-21(4)
C23	58(5)	77(6)	71(6)	1(5)	5(5)	-22(5)
C24	58(6)	80(7)	76(7)	0(6)	6(5)	-23(5)
C25	59(6)	81(7)	80(7)	-2(6)	9(5)	-25(5)
C26	58(5)	78(7)	76(7)	1(6)	9(5)	-24(5)
C27	57(5)	75(7)	69(6)	2(5)	7(5)	-22(5)
C28	59(6)	82(9)	86(9)	-4(7)	10(5)	-25(5)
O31	106(8)	122(8)	117(8)	-3(6)	-7(6)	20(6)
O32	102(8)	125(8)	120(8)	-7(6)	-7(6)	20(6)
C31	105(7)	121(7)	117(7)	-3(5)	-6(5)	17(5)
C32	106(7)	125(8)	125(8)	-8(6)	-11(6)	21(5)
C33	110(8)	130(9)	129(8)	-11(7)	-15(6)	24(6)
C34	111(8)	132(9)	134(9)	-12(7)	-17(6)	25(6)
C35	110(8)	131(9)	136(9)	-12(7)	-16(7)	25(7)
C36	109(8)	130(9)	134(9)	-11(7)	-13(6)	24(6)
C37	107(8)	128(8)	130(9)	-11(7)	-12(6)	22(6)
C38	111(8)	131(11)	140(11)	-10(9)	-17(7)	24(7)
O41	64(7)	102(8)	78(6)	7(5)	12(5)	-11(6)
O42	73(7)	107(7)	83(6)	2(5)	19(5)	-20(6)
C41	71(6)	101(6)	82(5)	5(4)	15(4)	-15(4)
C42	76(6)	117(7)	89(6)	-5(5)	23(5)	-25(5)
C43	79(7)	123(8)	92(7)	-9(6)	25(5)	-28(6)
C44	81(7)	127(8)	93(7)	-11(6)	27(6)	-31(6)

C45	81(7)	129(9)	94(7)	-12(7)	27(6)	-33(6)
C46	81(7)	129(9)	94(7)	-12(6)	28(6)	-33(6)
C47	80(6)	126(8)	93(7)	-10(6)	27(5)	-31(6)
C48	82(7)	130(10)	94(9)	-11(8)	27(7)	-33(7)
O51	45(7)	79(7)	67(7)	17(6)	-17(6)	-12(7)
O52	36(7)	72(7)	59(7)	5(6)	0(6)	-13(6)
C51	44(5)	69(5)	59(5)	4(4)	-5(4)	-13(4)
C52	34(6)	75(7)	61(6)	-1(6)	-7(5)	-30(6)
C53	36(7)	81(8)	69(7)	-2(7)	-5(7)	-34(7)
C54	35(7)	83(8)	75(8)	-2(7)	-2(7)	-39(7)
C55	35(7)	85(8)	81(8)	-3(7)	-8(7)	-40(7)
C56	34(7)	86(8)	74(8)	1(7)	-13(7)	-38(7)
C57	32(7)	81(8)	66(7)	3(7)	-11(6)	-33(7)
C58	39(9)	85(10)	89(10)	-4(9)	-3(9)	-38(8)
O61	91(9)	127(9)	108(9)	-1(8)	20(8)	16(8)
O62	80(9)	118(9)	101(9)	0(8)	19(8)	23(8)
C61	88(7)	117(7)	101(7)	-2(6)	11(5)	16(6)
C62	81(8)	124(9)	101(8)	-5(7)	4(7)	22(7)
C63	81(9)	128(10)	105(10)	-6(9)	0(9)	22(9)
C64	81(10)	130(11)	107(10)	-7(10)	-2(9)	25(9)
C65	81(10)	134(11)	112(10)	-8(10)	-1(9)	27(9)
C66	81(10)	134(11)	107(10)	-6(9)	1(9)	25(9)
C67	79(9)	128(10)	103(10)	-4(9)	2(9)	25(9)
C68	84(12)	137(13)	117(12)	-10(11)	-1(11)	26(11)

O71	46(7)	77(7)	71(7)	-10(7)	-17(6)	-41(6)
O72	38(7)	85(8)	55(7)	1(7)	-13(6)	-39(6)
C71	45(5)	77(6)	62(5)	-3(5)	-14(5)	-30(5)
C72	41(6)	82(7)	69(6)	-4(6)	-22(6)	-36(6)
C73	46(8)	92(8)	76(8)	-3(7)	-27(7)	-35(7)
C74	50(8)	97(9)	81(8)	-2(8)	-32(7)	-37(7)
C75	51(8)	95(9)	85(8)	-3(8)	-28(7)	-40(7)
C76	52(8)	91(9)	85(8)	0(8)	-21(7)	-41(7)
C77	45(8)	86(8)	79(8)	-2(7)	-22(7)	-40(7)
C78	52(10)	95(10)	89(10)	-1(9)	-26(9)	-38(9)
O81	54(8)	124(9)	77(8)	-1(8)	22(7)	20(7)
O82	63(8)	113(9)	94(9)	-6(8)	8(7)	30(7)
C81	64(6)	110(7)	87(7)	1(5)	12(5)	20(5)
C82	57(7)	115(8)	98(8)	4(7)	18(7)	29(7)
C83	57(9)	121(10)	107(9)	10(8)	17(8)	29(8)
C84	59(9)	125(10)	113(10)	9(9)	18(8)	31(8)
C85	61(9)	129(10)	116(10)	3(9)	24(8)	32(8)
C86	60(9)	127(10)	111(10)	4(9)	27(8)	32(8)
C87	58(9)	123(10)	105(9)	5(8)	24(8)	30(8)
C88	65(11)	134(12)	124(12)	2(11)	28(10)	28(10)

Table S5. Bond Lengths for ErSDC.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Er1	O1	2.46(3)	O42	C41	1.239(7)
Er1	O12	2.194(16)	C41	C42	1.524(10)
Er1	O22	2.338(14)	C42	C43	1.375(8)
Er1	O31	2.238(19)	C42	C47	1.377(8)
Er1	O41	2.278(14)	C43	C44	1.427(9)
Er1	O72[1]	2.277(13)	C44	C45	1.360(9)
Er1	O82[1]	2.203(16)	C45	C46	1.359(9)
Er2	O2	2.295(17)	C45	C48	1.485(12)
Er2	O3	2.37(2)	C46	C47	1.430(9)
Er2	O4	2.38(2)	C48	C68[4]	1.21(2)
Er2	O11	2.079(18)	O51	C51	1.236(7)
Er2	O21	2.262(13)	O52	C51	1.237(7)
Er2	O51	2.271(13)	C51	C52	1.521(10)
Er2	O61	2.189(18)	C52	C53	1.376(8)
Er3	O5	2.46(3)	C52	C57	1.374(8)
Er3	O32[2]	2.375(18)	C53	C54	1.427(9)
Er3	O42[2]	2.319(17)	C54	C55	1.359(9)
Er3	O52	2.358(13)	C55	C56	1.359(9)
Er3	O62	2.171(16)	C55	C58	1.486(12)
Er3	O71	2.315(12)	C56	C57	1.426(9)
Er3	O81	2.205(15)	C58	C78[6]	1.24(2)

O11	C11	1.240(7)	O61	C61	1.237(7)
O12	C11	1.240(7)	O62	C61	1.237(7)
C11	C12	1.523(10)	C61	C62	1.522(10)
C12	C13	1.376(8)	C62	C63	1.376(8)
C12	C17	1.376(8)	C62	C67	1.375(8)
C13	C14	1.427(9)	C63	C64	1.427(9)
C14	C15	1.358(9)	C64	C65	1.358(9)
C15	C16	1.360(9)	C65	C66	1.360(9)
C15	C18	1.485(12)	C65	C68	1.485(12)
C16	C17	1.426(9)	C66	C67	1.426(9)
C18	C38^{3}	1.23(2)	C68	C48^{7}	1.21(2)
O21	C21	1.239(7)	O71	C71	1.237(6)
O22	C21	1.239(7)	O72	Er1^{2}	2.278(13)
C21	C22	1.523(10)	O72	C71	1.239(6)
C22	C23	1.378(8)	C71	C72	1.520(10)
C22	C27	1.375(8)	C72	C73	1.377(8)
C23	C24	1.426(9)	C72	C77	1.375(8)
C24	C25	1.359(9)	C73	C74	1.426(9)
C25	C26	1.359(9)	C74	C75	1.359(9)
C25	C28	1.485(12)	C75	C76	1.358(9)
C26	C27	1.428(9)	C75	C78	1.485(12)
C28	C88^{4}	1.18(2)	C76	C77	1.427(9)
O31	C31	1.239(7)	C78	C58^{8}	1.24(2)
O32	Er3^{1}	2.375(18)	O81	C81	1.241(7)

O32	C31	1.239(7)	O82	Er1[2]	2.203(16)
C31	C32	1.522(10)	O82	C81	1.239(7)
C32	C33	1.375(8)	C81	C82	1.523(10)
C32	C37	1.374(8)	C82	C83	1.375(8)
C33	C34	1.427(9)	C82	C87	1.376(8)
C34	C35	1.359(9)	C83	C84	1.426(9)
C35	C36	1.359(9)	C84	C85	1.358(9)
C35	C38	1.486(12)	C85	C86	1.358(9)
C36	C37	1.428(9)	C85	C88	1.485(12)
C38	C18[5]	1.23(2)	C86	C87	1.427(9)
O41	C41	1.240(7)	C88	C28[7]	1.18(2)
O42	Er3[1]	2.319(17)			

[1]+X,1-Y,-1/2+Z; [2]+X,1-Y,1/2+Z; [3]-1/2+X,1/2+Y,+Z; [4]1/2+X,3/2-Y,-1/2+Z; [5]1/2+X,-1/2+Y,+Z; [6]1/2+X,1/2+Y,+Z; [7]-1/2+X,3/2-Y,1/2+Z; [8]-1/2+X,-1/2+Y,+Z

Table S6. Bond Angles for ErSDC.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O12	Er1	O1	79.0(8)	C31	O32	Er3[1]	138.3(15)
O12	Er1	O22	85.1(7)	O31	C31	O32	129.2(18)
O12	Er1	O31	129.7(7)	O31	C31	C32	117.2(16)
O12	Er1	O41	151.2(6)	O32	C31	C32	113.5(16)
O12	Er1	O72[1]	88.4(7)	C33	C32	C31	119.0(17)
O12	Er1	O82[1]	82.9(6)	C37	C32	C31	122.3(17)
O22	Er1	O1	75.7(7)	C37	C32	C33	118.8(17)
O31	Er1	O1	127.7(9)	C32	C33	C34	122(2)
O31	Er1	O22	66.7(7)	C35	C34	C33	120(2)
O31	Er1	O41	74.5(6)	C34	C35	C38	115.7(19)
O31	Er1	O72[1]	134.1(6)	C36	C35	C34	118.5(19)
O41	Er1	O1	72.7(8)	C36	C35	C38	126(2)
O41	Er1	O22	93.2(7)	C35	C36	C37	123(2)
O72[1]	Er1	O1	77.8(8)	C32	C37	C36	118.3(19)
O72[1]	Er1	O22	153.4(5)	C18[5]	C38	C35	131(3)
O72[1]	Er1	O41	80.4(6)	C41	O41	Er1	157.1(15)
O82[1]	Er1	O1	153.8(9)	C41	O42	Er3[1]	119.9(12)
O82[1]	Er1	O22	121.6(6)	O41	C41	C42	113.6(14)
O82[1]	Er1	O31	78.6(7)	O42	C41	O41	133.3(16)
O82[1]	Er1	O41	121.4(7)	O42	C41	C42	113.1(14)
O82[1]	Er1	O72[1]	82.9(6)	C43	C42	C41	118.7(15)

O2	Er2	O3	147.8(8)	C43	C42	C47	119.3(16)
O2	Er2	O4	149.6(8)	C47	C42	C41	122.0(15)
O3	Er2	O4	61.3(8)	C42	C43	C44	119.4(18)
O11	Er2	O2	81.8(5)	C45	C44	C43	121.6(19)
O11	Er2	O3	102.2(6)	C44	C45	C48	116.7(17)
O11	Er2	O4	102.9(7)	C46	C45	C44	118.9(18)
O11	Er2	O21	88.9(7)	C46	C45	C48	124.4(18)
O11	Er2	O51	158.5(6)	C45	C46	C47	120.9(19)
O11	Er2	O61	82.8(8)	C42	C47	C46	119.9(17)
O21	Er2	O2	83.2(5)	C68[4]	C48	C45	122(2)
O21	Er2	O3	65.1(7)	C51	O51	Er2	160.2(13)
O21	Er2	O4	126.4(7)	C51	O52	Er3	145.8(9)
O21	Er2	O51	89.5(6)	O51	C51	O52	123.9(14)
O51	Er2	O2	76.7(5)	O51	C51	C52	116.1(12)
O51	Er2	O3	96.6(7)	O52	C51	C52	120.0(13)
O51	Er2	O4	95.3(6)	C53	C52	C51	124.9(13)
O61	Er2	O2	85.4(5)	C57	C52	C51	115.8(12)
O61	Er2	O3	126.7(7)	C57	C52	C53	119.3(14)
O61	Er2	O4	65.9(7)	C52	C53	C54	121.6(16)
O61	Er2	O21	166.7(6)	C55	C54	C53	118.7(16)
O61	Er2	O51	94.4(7)	C54	C55	C58	122.3(16)
O32[2]	Er3	O5	67.3(8)	C56	C55	C54	120.1(15)
O42[2]	Er3	O5	125.4(9)	C56	C55	C58	117.7(15)
O42[2]	Er3	O32[2]	85.8(6)	C55	C56	C57	122.0(16)

O42[2]	Er3	O52	57.7(5)	C52	C57	C56	118.4(15)
O52	Er3	O5	77.9(8)	C78[6]	C58	C55	133(2)
O52	Er3	O32[2]	95.7(7)	C61	O61	Er2	151.2(18)
O62	Er3	O5	77.0(8)	C61	O62	Er3	168.2(14)
O62	Er3	O32[2]	142.5(6)	O61	C61	C62	114.2(15)
O62	Er3	O42[2]	125.9(7)	O62	C61	O61	128.0(19)
O62	Er3	O52	87.6(7)	O62	C61	C62	117.8(16)
O62	Er3	O71	86.7(6)	C63	C62	C61	117.7(16)
O62	Er3	O81	92.5(8)	C67	C62	C61	122.5(16)
O71	Er3	O5	156.7(9)	C67	C62	C63	119.8(17)
O71	Er3	O32[2]	123.1(6)	C62	C63	C64	121.1(19)
O71	Er3	O42[2]	77.7(6)	C65	C64	C63	119.3(19)
O71	Er3	O52	118.3(5)	C64	C65	C66	119.3(19)
O81	Er3	O5	84.2(8)	C64	C65	C68	119.7(18)
O81	Er3	O32[2]	73.2(7)	C66	C65	C68	121(2)
O81	Er3	O42[2]	133.6(6)	C65	C66	C67	123(2)
O81	Er3	O52	161.6(6)	C62	C67	C66	117.7(18)
O81	Er3	O71	80.1(6)	C48[7]	C68	C65	133(3)
C11	O11	Er2	152.3(17)	C71	O71	Er3	144.7(11)
C11	O12	Er1	174.0(16)	C71	O72	Er1[2]	135.8(11)
O11	C11	O12	125.1(18)	O71	C71	O72	126.3(14)
O11	C11	C12	119.6(15)	O71	C71	C72	115.5(12)
O12	C11	C12	115.3(15)	O72	C71	C72	118.2(12)
C13	C12	C11	121.0(16)	C73	C72	C71	117.9(12)

C17	C12	C11	119.3(15)	C77	C72	C71	118.8(12)
C17	C12	C13	119.6(17)	C77	C72	C73	123.3(14)
C12	C13	C14	120.0(18)	C72	C73	C74	117.3(15)
C15	C14	C13	121.2(19)	C75	C74	C73	120.1(16)
C14	C15	C16	118.1(18)	C74	C75	C78	117.7(15)
C14	C15	C18	119.7(19)	C76	C75	C74	121.8(16)
C16	C15	C18	122.2(19)	C76	C75	C78	120.5(16)
C15	C16	C17	122.7(19)	C75	C76	C77	120.0(16)
C12	C17	C16	118.4(18)	C72	C77	C76	117.5(15)
C38[3]	C18	C15	129(3)	C58[8]	C78	C75	125(2)
C21	O21	Er2	148.7(11)	C81	O81	Er3	146.2(14)
C21	O22	Er1	138.6(10)	C81	O82	Er1[2]	134.0(14)
O21	C21	O22	129.7(16)	O81	C81	C82	114.4(14)
O21	C21	C22	114.3(13)	O82	C81	O81	131.3(16)
O22	C21	C22	116.0(13)	O82	C81	C82	114.3(14)
C23	C22	C21	118.1(13)	C83	C82	C81	119.2(15)
C27	C22	C21	120.0(13)	C83	C82	C87	121.3(15)
C27	C22	C23	121.9(15)	C87	C82	C81	119.5(15)
C22	C23	C24	120.0(16)	C82	C83	C84	117.3(17)
C25	C24	C23	117.4(17)	C85	C84	C83	122.4(18)
C24	C25	C28	113.2(15)	C84	C85	C88	117.3(18)
C26	C25	C24	123.4(16)	C86	C85	C84	119.5(17)
C26	C25	C28	123.4(17)	C86	C85	C88	123.2(19)
C25	C26	C27	119.8(17)	C85	C86	C87	120.1(18)

C22	C27	C26	117.5(16)	C82	C87	C86	119.4(17)
C88[4]	C28	C25	145(3)	C28[7]	C88	C85	144(3)
C31	O31	Er1	137.7(16)				

[1]+X,1-Y,-1/2+Z; [2]+X,1-Y,1/2+Z; [3]-1/2+X,1/2+Y,+Z; [4]1/2+X,3/2-Y,-1/2+Z; [5]1/2+X,-1/2+Y,+Z; [6]1/2+X,1/2+Y,+Z; [7]-1/2+X,3/2-Y,1/2+Z; [8]-1/2+X,-1/2+Y,+Z

Table S7. Torsion Angles for ErSDC.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
Er1	O22	C21	O21	57.0(16)	O41	C41	C42	C47	180.0(5)
Er1	O22	C21	C22	-123.1(16)	O42	C41	C42	C43	179.9(4)
Er1	O31	C31	O32	-27.7(16)	O42	C41	C42	C47	-0.1(6)
Er1	O31	C31	C32	152.4(16)	C41	C42	C43	C44	179.8(5)
Er1	O41	C41	O42	10(3)	C41	C42	C47	C46	-179.7(5)
Er1	O41	C41	C42	-170(3)	C42	C43	C44	C45	0.1(9)
Er1[1]	O72	C71	O71	20.8(10)	C43	C42	C47	C46	0.3(9)
Er1[1]	O72	C71	C72	-159.2(10)	C43	C44	C45	C46	-0.1(10)
Er1[1]	O82	C81	O81	-16.7(12)	C43	C44	C45	C48	179.9(6)
Er1[1]	O82	C81	C82	163.4(12)	C44	C45	C46	C47	0.2(9)
Er2	O11	C11	O12	2.5(17)	C44	C45	C48	C68[4]	156(3)
Er2	O11	C11	C12	-177.5(17)	C45	C46	C47	C42	-0.3(9)
Er2	O21	C21	O22	40(2)	C46	C45	C48	C68[4]	-24(3)
Er2	O21	C21	C22	-140(2)	C47	C42	C43	C44	-0.3(9)
Er2	O51	C51	O52	29(2)	C48	C45	C46	C47	-179.9(6)
Er2	O51	C51	C52	-151(2)	O51	C51	C52	C53	-0.1(6)
Er2	O61	C61	O62	-19.0(19)	O51	C51	C52	C57	-179.8(4)
Er2	O61	C61	C62	161.1(19)	O52	C51	C52	C53	-180.0(4)
Er3[2]	O32	C31	O31	34.8(17)	O52	C51	C52	C57	0.2(5)
Er3[2]	O32	C31	C32	-145.3(17)	C51	C52	C53	C54	-179.8(4)
Er3[2]	O42	C41	O41	-16.8(8)	C51	C52	C57	C56	180.0(4)

Er3[2] O42 C41 C42	163.3(8)	C52 C53 C54 C55	-0.1(8)
Er3 O52 C51 O51	-68(2)	C53 C52 C57 C56	0.2(8)
Er3 O52 C51 C52	112(2)	C53 C54 C55 C56	0.0(8)
Er3 O62 C61 O61	48(7)	C53 C54 C55 C58	-179.7(5)
Er3 O62 C61 C62	-133(7)	C54 C55 C56 C57	0.2(9)
Er3 O71 C71 O72	-37.1(15)	C54 C55 C58 C78[6]	-28(3)
Er3 O71 C71 C72	142.9(15)	C55 C56 C57 C52	-0.3(8)
Er3 O81 C81 O82	16.2(17)	C56 C55 C58 C78[6]	152(3)
Er3 O81 C81 C82	-163.9(18)	C57 C52 C53 C54	0.0(8)
O11 C11 C12 C13	0.1(6)	C58 C55 C56 C57	179.9(5)
O11 C11 C12 C17	-180.0(4)	O61 C61 C62 C63	-0.3(6)
O12 C11 C12 C13	-179.9(4)	O61 C61 C62 C67	-180.0(4)
O12 C11 C12 C17	0.0(5)	O62 C61 C62 C63	179.8(4)
C11 C12 C13 C14	-179.8(4)	O62 C61 C62 C67	0.1(6)
C11 C12 C17 C16	180.0(4)	C61 C62 C63 C64	180.0(5)
C12 C13 C14 C15	-0.3(8)	C61 C62 C67 C66	179.8(5)
C13 C12 C17 C16	-0.2(8)	C62 C63 C64 C65	0.3(9)
C13 C14 C15 C16	0.2(8)	C63 C62 C67 C66	0.1(8)
C13 C14 C15 C18	-179.6(5)	C63 C64 C65 C66	0.0(9)
C14 C15 C16 C17	-0.1(9)	C63 C64 C65 C68	179.7(5)
C14 C15 C18 C38[3]	40(3)	C64 C65 C66 C67	-0.2(9)
C15 C16 C17 C12	0.1(8)	C64 C65 C68 C48[7]	153(3)
C16 C15 C18 C38[3]	-140(3)	C65 C66 C67 C62	0.1(9)
C17 C12 C13 C14	0.3(8)	C66 C65 C68 C48[7]	-27(3)

C18 C15 C16 C17	179.8(5)	C67 C62 C63 C64	-0.3(9)
O21 C21 C22 C23	-0.2(6)	C68 C65 C66 C67	-179.9(5)
O21 C21 C22 C27	180.0(4)	O71 C71 C72 C73	0.0(5)
O22 C21 C22 C23	179.8(4)	O71 C71 C72 C77	179.8(4)
O22 C21 C22 C27	0.0(6)	O72 C71 C72 C73	-180.0(4)
C21 C22 C23 C24	179.9(5)	O72 C71 C72 C77	-0.2(6)
C21 C22 C27 C26	179.8(5)	C71 C72 C73 C74	-179.9(4)
C22 C23 C24 C25	0.3(9)	C71 C72 C77 C76	179.9(4)
C23 C22 C27 C26	0.0(9)	C72 C73 C74 C75	-0.2(8)
C23 C24 C25 C26	0.0(9)	C73 C72 C77 C76	-0.3(9)
C23 C24 C25 C28	179.9(5)	C73 C74 C75 C76	0.0(9)
C24 C25 C26 C27	-0.3(9)	C73 C74 C75 C78	180.0(5)
C24 C25 C28 C88[4]	177(3)	C74 C75 C76 C77	0.0(9)
C25 C26 C27 C22	0.3(9)	C74 C75 C78 C58[8]	-148(2)
C26 C25 C28 C88[4]	-3(4)	C75 C76 C77 C72	0.2(8)
C27 C22 C23 C24	-0.3(9)	C76 C75 C78 C58[8]	32(2)
C28 C25 C26 C27	179.8(5)	C77 C72 C73 C74	0.3(9)
O31 C31 C32 C33	-0.3(6)	C78 C75 C76 C77	-180.0(5)
O31 C31 C32 C37	-180.0(4)	O81 C81 C82 C83	0.0(6)
O32 C31 C32 C33	179.8(4)	O81 C81 C82 C87	179.9(4)
O32 C31 C32 C37	0.1(6)	O82 C81 C82 C83	179.9(4)
C31 C32 C33 C34	-179.9(5)	O82 C81 C82 C87	-0.1(6)
C31 C32 C37 C36	179.8(5)	C81 C82 C83 C84	179.9(5)
C32 C33 C34 C35	0.3(9)	C81 C82 C87 C86	-179.7(5)

C33 C32 C37 C36	0.1(9)	C82 C83 C84 C85	-0.1(9)
C33 C34 C35 C36	-0.2(9)	C83 C82 C87 C86	0.2(9)
C33 C34 C35 C38	179.9(5)	C83 C84 C85 C86	0.1(9)
C34 C35 C36 C37	0.1(9)	C83 C84 C85 C88	179.9(6)
C34 C35 C38 C18[5]	171(3)	C84 C85 C86 C87	0.1(9)
C35 C36 C37 C32	0.0(9)	C84 C85 C88 C28[7]	144(4)
C36 C35 C38 C18[5]	-9(3)	C85 C86 C87 C82	-0.2(9)
C37 C32 C33 C34	-0.2(9)	C86 C85 C88 C28[7]	-36(4)
C38 C35 C36 C37	180.0(6)	C87 C82 C83 C84	-0.1(9)
O41 C41 C42 C43	0.0(6)	C88 C85 C86 C87	-179.8(6)

[1]+X,1-Y,1/2+Z; [2]+X,1-Y,-1/2+Z; [3]-1/2+X,1/2+Y,+Z; [4]1/2+X,3/2-Y,-1/2+Z; [5]1/2+X,-1/2+Y,+Z; [6]1/2+X,1/2+Y,+Z; [7]-1/2+X,3/2-Y,1/2+Z; [8]-1/2+X,-1/2+Y,+Z

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for ErSDC.

Atom	*X*	*y*	*z*	U(eq)
H13	3696	7497	2088	120
H14	2959	7718	1880	123
H16	3153	6767	496	122
H17	3893	6527	684	119
H18	2376	7003	859	127
H23	6128	7877	1977	82
H24	6867	8300	1885	86
H26	7031	6580	793	85
H27	6295	6139	883	81
H28	7477	8229	1530	91
H33	6117	4659	1228	148
H34	6801	4164	1498	150
H36	6777	2517	368	149
H37	6092	2993	88	146
H38	7407	3371	1407	153
H43	6068	6837	60	117
H44	6732	7514	-113	120
H46	6850	6296	-1431	122
H47	6185	5607	-1273	119
H48	7304	7943	-689	122

H53	6251	7578	2945	75
H54	6961	8030	3151	77
H56	6936	6614	4403	77
H57	6227	6147	4204	72
H58	7504	7593	4311	85
H63	3786	7546	2929	126
H64	3067	8005	3072	127
H66	3095	6972	4458	129
H67	3813	6497	4328	124
H68	2488	8297	3691	136
H73	3987	4456	3727	86
H74	3318	3961	3381	91
H76	3181	2404	4559	91
H77	3848	2877	4923	84
H78	2762	2857	3351	94
H83	3929	6924	5025	114
H84	3280	7548	5326	119
H86	3254	6069	6545	119
H87	3904	5426	6263	114
H88	2831	7863	6022	129

Experimental

Single crystals of $C_{64}H_{40}Er_3O_{21}$ **[ErSDC]** were crystallised solvothermally. A suitable crystal was selected and **[]** on a **Bruker APEXII** diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2 [1], the structure was solved with the XT [2] structure solution program using Intrinsic Phasing and refined with the XL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

Crystal structure determination of [ErSDC]

Crystal Data for $C_{64}H_{40}Er_3O_{21}$ (M =1646.74 g/mol): monoclinic, space group Cc (no. 9), a = 30.6336(8) Å, b = 16.0923(6) Å, c = 25.8791(10) Å, β = 90°, V = 12757.4(8) Å^3, Z = 4, T = 100(2) K, μ(MoKα) = 1.992 mm^{-1}, *Dcalc* = 0.857 g/cm^3, 36038 reflections measured (3.09° ≤ 2Θ ≤ 50.054°), 18590 unique (R_{int} = 0.0489, R_{sigma} = 0.0691) which were used in all calculations. The final R_1 was 0.0803 (I > 2σ(I)) and wR_2 was 0.2307 (all data).

Refinement model description

Number of restraints - 2131, number of constraints none.

Details:

```
1. Twinned data refinement
 Scales: 0.35(4) 0.17(2) 0.29(2) 0.19(2)
2. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
3. Restrained distances
 Er3-O5
 2.34 with sigma of 0.05
 Er1-O1
 2.34 with sigma of 0.05
 Er2-O3
 2.34 with sigma of 0.02
 Er2-O4
 2.34 with sigma of 0.02
 O3-O4
 2.5 with sigma of 0.02
 Er2-O2
 2.34 with sigma of 0.05
 C18-C38_$1 ≈ C28-C88_$2 ≈ C48-C68_$2 ≈ C58-C78_$3
 with sigma of 0.02
 O5-O62 ≈ O5-O32_$4
 with sigma of 0.05
 O5-O52 ≈ O5-O81
 with sigma of 0.05
 O1-O12 ≈ O1-O41
 with sigma of 0.05
 O1-O22 ≈ O1-O72_$5
 with sigma of 0.05
 O3-O21 ≈ O4-O61
 with sigma of 0.02
 O3-O11 ≈ O3-O51 ≈ O4-O11 ≈ O4-O51
 with sigma of 0.02
 O2-O11 ≈ O2-O51
 with sigma of 0.02
 O2-O21 ≈ O2-O61
 with sigma of 0.02
4. Restrained planarity
 O11, O12, C11, C12, C13, C14, C15, C16, C17, C18
 with sigma of 0.005
```

O21, O22, C21, C22, C23, C24, C25, C26, C27, C28
with sigma of 0.005
O31, O32, C31, C32, C33, C34, C35, C36, C37, C38
with sigma of 0.005
O41, O42, C41, C42, C43, C44, C45, C46, C47, C48
with sigma of 0.005
O51, O52, C51, C52, C53, C54, C55, C56, C57, C58
with sigma of 0.005
O61, O62, C61, C62, C63, C64, C65, C66, C67, C68
with sigma of 0.005
O71, O72, C71, C72, C73, C74, C75, C76, C77, C78
with sigma of 0.005
O81, O82, C81, C82, C83, C84, C85, C86, C87, C88
with sigma of 0.005
5. Uiso/Uaniso restraints and constraints
All non-hydrogen atoms have similar U: within 2A with sigma of 0.005 and sigma for terminal atoms of 0.01
Uanis(C11) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(C41) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(C21) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(C31) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(O1) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(O3) ≈ Ueq, Uanis(O4) ≈ Ueq: with sigma of 0.0045 and sigma for terminal atoms of 0.009
Uanis(O2) ≈ Ueq: with sigma of 0.005 and sigma for terminal atoms of 0.01
Uanis(C61) ≈ Ueq, Uanis(C71) ≈ Ueq, Uanis(C81) ≈ Ueq: with sigma of 0.005 and sigma for terminal atoms of 0.01
Uanis(C51) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(O1) = Uanis(O5)
Uanis(O3) = Uanis(O4)
6. Rigid body (RIGU) restrains
O11, O12, C11, C12, C13, C14, C15, C16, C17, C18
with sigma for 1-2 distances of 0.001 and sigma for 1-3 distances of 0.001
O41, O42, C41, C42, C43, C44, C45, C46, C47, C48
with sigma for 1-2 distances of 0.001 and sigma for 1-3 distances of 0.001
O21, O22, C21, C22, C23, C24, C25, C26, C27, C28
with sigma for 1-2 distances of 0.001 and sigma for 1-3 distances of 0.001
O31, O32, C31, C32, C33, C34, C35, C36, C37, C38
with sigma for 1-2 distances of 0.001 and sigma for 1-3 distances of 0.001
7. Same fragment restrains
{O12, O11, C11, C12, C17, C16, C15, C14, C13, C18} sigma for 1-2: 0.005, 1-3: 0.04
{O21, O22, C21, C22, C23, C24, C25, C26, C27, C28} sigma for 1-2: 0.005, 1-3: 0.04
{O31, O32, C31, C32, C33, C34, C35, C36, C37, C38} sigma for 1-2: 0.005, 1-3: 0.04
{O41, O42, C41, C42, C43, C44, C45, C46, C47, C48} sigma for 1-2: 0.005, 1-3: 0.04
{O51, O52, C51, C52, C53, C54, C55, C56, C57, C58} sigma for 1-2: 0.005, 1-3: 0.04
{O61, O62, C61, C62, C63, C64, C65, C66, C67, C68} sigma for 1-2: 0.005, 1-3: 0.04
{O71, O72, C71, C72, C73, C74, C75, C76, C77, C78} sigma for 1-2: 0.005, 1-3: 0.04
{O81, O82, C81, C82, C83, C84, C85, C86, C87, C88} sigma for 1-2: 0.005, 1-3: 0.04
as
{O11, O12, C11, C12, C13, C14, C15, C16, C17, C18}
8.a Aromatic/amide H refined with riding coordinates:
C13(H13), C14(H14), C16(H16), C17(H17), C18(H18), C23(H23), C24(H24),
C26(H26), C27(H27), C28(H28), C33(H33), C34(H34), C36(H36), C37(H37), C38(H38),
C43(H43), C44(H44), C46(H46), C47(H47), C48(H48), C53(H53), C54(H54),
C56(H56), C57(H57), C58(H58), C63(H63), C64(H64), C66(H66), C67(H67), C68(H68),

C73(H73), C74(H74), C76(H76), C77(H77), C78(H78), C83(H83), C84(H84), C86(H86), C87(H87), C88(H88)

This report has been created with Olex2, compiled on 2016.08.25 svn.r3337 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

TmSDC

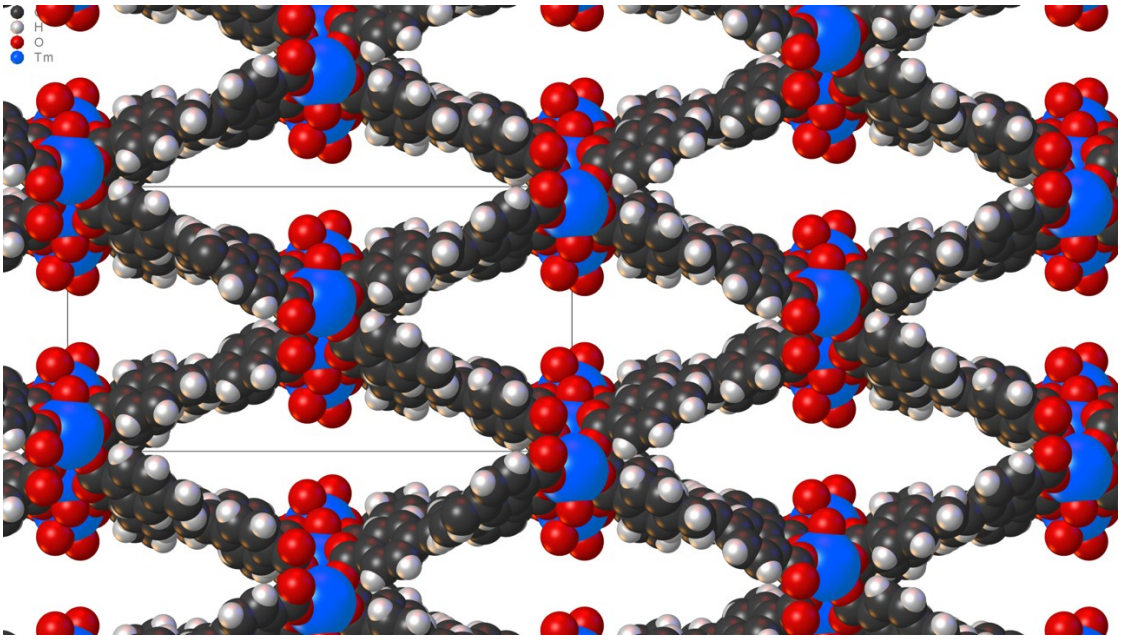

Table S9. Crystal data and structure refinement for TmSDC.

Identification code	TmSDC
Empirical formula	$C_{64}H_{40}O_{21}Tm_3$
Formula weight	1651.75
Temperature/K	100(2)
Crystal system	monoclinic
Space group	Cc
a/Å	30.4920(8)
b/Å	15.9861(7)
c/Å	25.7022(13)

α/°	90
β/°	89.991(3)
γ/°	90
Volume/Å^3	12528.5(9)
Z	4
ρ_{calc}g/cm^3	0.876
μ/mm^{-1}	2.144
F(000)	3196.0
Crystal size/mm^3	0.228 × 0.205 × 0.16
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.144 to 50.048
Index ranges	-35 ≤ h ≤ 36, -19 ≤ k ≤ 19, -30 ≤ l ≤ 30
Reflections collected	34959
Independent reflections	19378 [R_{int} = 0.0404, R_{sigma} = 0.0541]
Data/restraints/parameters	19378/2125/784
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0745, wR_2 = 0.1910
Final R indexes [all data]	R_1 = 0.0914, wR_2 = 0.2053
Largest diff. peak/hole / e Å^{-3}	1.99/-0.95
Flack parameter	?

Table S10. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for TmSDC. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*y*	*z*	U(eq)
Tm1	4998.9(7)	5977.2(6)	636.6(11)	61.3(3)
Tm2	5004.3(9)	7080.6(9)	2511.1(12)	77.4(4)
Tm3	4997.0(8)	5690.9(6)	4375.1(11)	58.6(3)
O1	5145(12)	7530(20)	540(12)	199(11)
O2	5030(7)	5668(10)	2374(6)	92(6)
O3	5253(8)	8406(15)	2275(9)	240(17)
O4	4754(8)	8227(16)	3012(9)	240(17)
O5	5056(13)	7150(20)	4395(12)	199(11)
O11	4472(6)	6982(8)	1987(6)	74(4)
O12	4574(6)	6425(8)	1232(7)	76(4)
C11	4334(5)	6787(5)	1550(5)	75(3)
C12	3865(5)	7006(8)	1418(7)	78(3)
C13	3590(6)	7405(10)	1756(8)	81(4)
C14	3151(6)	7598(12)	1617(8)	83(4)
C15	2995(6)	7391(11)	1144(8)	85(4)
C16	3258(6)	6997(11)	803(9)	84(4)
C17	3698(6)	6805(10)	942(8)	82(4)
C18	2527(6)	7626(14)	1036(11)	85(5)
O21	5490(5)	7206(8)	1837(5)	64(3)
O22	5555(5)	6210(7)	1217(5)	56(3)
C21	5684(4)	6787(6)	1502(3)	61(3)

C22	6160(4)	7043(9)	1442(5)	63(3)
C23	6333(6)	7674(10)	1736(7)	65(3)
C24	6780(6)	7909(11)	1677(7)	66(3)
C25	7030(6)	7507(10)	1324(7)	69(3)
C26	6871(6)	6884(11)	1027(7)	66(3)
C27	6424(5)	6649(11)	1090(6)	65(3)
C28	7499(6)	7781(14)	1280(9)	73(4)
O31	5408(6)	4784(9)	633(7)	86(4)
O32	5455(6)	3764(10)	54(5)	85(4)
C31	5595(4)	4181(7)	427(4)	84(3)
C32	6035(4)	3920(10)	645(6)	85(3)
C33	6214(6)	4344(12)	1055(7)	87(4)
C34	6629(6)	4073(13)	1244(8)	86(4)
C35	6843(6)	3421(11)	1031(8)	87(4)
C36	6666(6)	3002(13)	628(8)	87(4)
C37	6252(6)	3258(12)	431(8)	86(4)
C38	7280(7)	3150(15)	1241(10)	86(5)
O41	5463(6)	5975(10)	-75(5)	77(4)
O42	5556(6)	5203(9)	-800(6)	87(4)
C41	5657(4)	5740(6)	-472(4)	83(3)
C42	6087(4)	6186(10)	-570(7)	89(4)
C43	6248(6)	6793(12)	-250(8)	92(4)
C44	6654(6)	7193(14)	-357(9)	94(4)
C45	6898(7)	6995(12)	-777(8)	94(4)

C46	6747(7)	6397(13)	-1099(9)	95(4)
C47	6340(6)	5998(13)	-992(8)	95(4)
C48	7323(7)	7453(16)	-856(11)	94(5)
O51	5549(6)	6771(10)	3039(5)	83(4)
O52	5505(6)	5934(9)	3713(6)	80(4)
C51	5702(4)	6447(6)	3438(4)	79(4)
C52	6160(4)	6740(9)	3564(6)	77(4)
C53	6378(5)	7307(11)	3261(8)	78(4)
C54	6810(6)	7577(13)	3381(8)	77(4)
C55	6997(6)	7253(11)	3811(8)	77(4)
C56	6792(5)	6694(12)	4117(8)	74(4)
C57	6361(5)	6424(11)	3995(7)	76(4)
C58	7453(6)	7508(15)	3966(10)	78(5)
O61	4521(7)	6876(10)	3125(6)	99(5)
O62	4507(7)	6149(9)	3857(7)	94(5)
C61	4343(5)	6621(6)	3529(5)	94(4)
C62	3880(5)	6924(9)	3621(8)	91(4)
C63	3692(7)	7446(12)	3264(9)	91(5)
C64	3257(7)	7736(14)	3343(9)	91(5)
C65	3033(7)	7498(12)	3769(9)	93(5)
C66	3211(7)	6984(13)	4127(9)	92(5)
C67	3646(7)	6691(13)	4049(8)	91(5)
C68	2576(7)	7844(16)	3814(11)	95(6)
O71	4607(5)	4456(8)	4295(6)	65(4)

O72	4539(5)	3630(9)	5001(5)	64(4)
C71	4425(4)	3929(6)	4576(4)	64(3)
C72	3995(4)	3609(8)	4359(6)	69(3)
C73	3845(5)	3903(11)	3894(7)	76(4)
C74	3440(5)	3596(12)	3696(8)	81(4)
C75	3213(5)	3024(11)	3968(7)	82(4)
C76	3366(6)	2737(12)	4425(8)	79(4)
C77	3768(5)	3026(10)	4638(7)	74(4)
C78	2788(6)	2724(15)	3736(10)	85(5)
O81	4544(6)	5860(10)	5010(5)	82(5)
O82	4537(6)	5111(9)	5755(7)	95(5)
C81	4400(4)	5636(7)	5440(4)	88(4)
C82	3986(4)	6074(10)	5618(8)	95(4)
C83	3810(6)	6663(13)	5296(9)	101(5)
C84	3420(7)	7079(14)	5454(10)	105(5)
C85	3216(7)	6918(13)	5907(9)	106(5)
C86	3389(7)	6337(14)	6225(10)	103(5)
C87	3779(6)	5909(13)	6078(9)	99(5)
C88	2808(7)	7419(17)	6010(12)	111(6)

Table S11. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for TmSDC. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Tm1	31.6(5)	80.1(6)	72.2(6)	23.0(5)	0.2(11)	13.8(8)
Tm2	34.4(5)	127.5(11)	70.3(5)	-7.1(6)	0.6(11)	-15.5(11)
Tm3	30.6(5)	75.1(6)	70.1(6)	-27.1(5)	3.9(11)	-19.0(7)
O1	201(15)	210(14)	186(13)	12(10)	-9(11)	-14(11)
O2	87(11)	72(9)	116(12)	28(8)	14(12)	-32(10)
O3	243(19)	235(18)	242(18)	-7(9)	10(9)	-7(9)
O4	243(19)	235(18)	242(18)	-7(9)	10(9)	-7(9)
O5	201(15)	210(14)	186(13)	12(10)	-9(11)	-14(11)
O11	78(6)	70(7)	73(5)	3(5)	-17(4)	1(5)
O12	78(6)	76(7)	74(6)	2(5)	-17(5)	5(5)
C11	77(5)	74(5)	74(5)	1(4)	-16(4)	3(4)
C12	78(5)	77(6)	80(6)	-2(5)	-19(4)	5(4)
C13	79(5)	79(7)	84(6)	-5(5)	-18(5)	4(5)
C14	80(6)	80(8)	89(7)	-9(6)	-20(5)	5(5)
C15	82(6)	82(8)	90(7)	-10(6)	-22(5)	8(5)
C16	83(6)	83(8)	88(7)	-8(6)	-23(5)	10(5)
C17	82(6)	81(7)	83(6)	-5(5)	-22(5)	9(5)
C18	83(6)	80(10)	92(8)	-14(8)	-23(5)	8(6)
O21	55(5)	60(6)	77(6)	-1(5)	-4(5)	-15(4)
O22	49(5)	52(5)	68(6)	8(4)	-10(5)	-7(4)
C21	54(4)	58(4)	70(5)	3(4)	-7(4)	-11(3)

C22	54(4)	64(5)	72(6)	2(4)	-7(4)	-14(3)
C23	55(5)	65(6)	75(6)	1(5)	-8(4)	-14(4)
C24	55(5)	66(6)	78(7)	0(5)	-8(4)	-15(4)
C25	56(5)	69(6)	81(7)	-3(5)	-7(5)	-15(4)
C26	54(5)	66(6)	76(7)	1(5)	-7(4)	-14(4)
C27	54(5)	67(6)	74(6)	0(5)	-7(4)	-13(4)
C28	57(5)	73(8)	90(9)	-4(7)	-5(5)	-16(5)
O31	86(6)	84(6)	89(7)	9(5)	-17(5)	17(5)
O32	80(7)	86(6)	90(6)	7(5)	-19(5)	18(5)
C31	81(5)	83(5)	87(5)	9(4)	-17(4)	14(4)
C32	84(5)	81(6)	90(6)	6(5)	-21(5)	17(4)
C33	86(6)	81(6)	93(7)	5(5)	-24(5)	19(5)
C34	87(6)	78(7)	94(7)	4(6)	-25(5)	19(5)
C35	85(6)	78(7)	97(7)	2(6)	-26(6)	18(5)
C36	84(6)	81(7)	96(7)	1(6)	-24(5)	17(5)
C37	83(6)	82(6)	93(7)	3(6)	-23(5)	17(5)
C38	86(7)	75(8)	98(9)	0(7)	-27(6)	19(6)
O41	67(6)	81(7)	84(6)	12(5)	2(5)	-6(5)
O42	79(7)	90(6)	92(6)	5(5)	7(5)	-13(5)
C41	74(5)	86(5)	88(5)	7(4)	8(4)	-10(4)
C42	78(5)	95(6)	95(6)	-2(5)	15(5)	-17(5)
C43	78(6)	100(7)	98(7)	-6(6)	17(5)	-19(5)
C44	79(6)	102(7)	101(7)	-7(6)	18(5)	-21(6)
C45	79(6)	103(8)	101(8)	-8(6)	18(6)	-21(6)

C46	81(6)	103(8)	101(7)	-8(6)	19(5)	-22(6)
C47	81(6)	103(7)	100(7)	-7(6)	18(5)	-21(5)
C48	79(7)	101(9)	102(9)	-6(8)	17(6)	-20(6)
O51	44(8)	121(10)	83(9)	13(8)	-38(7)	-17(8)
O52	46(8)	109(10)	83(9)	15(8)	-13(7)	-18(8)
C51	44(7)	109(9)	83(8)	14(7)	-26(6)	-20(6)
C52	43(7)	99(8)	88(8)	10(7)	-25(6)	-24(6)
C53	43(7)	98(9)	94(9)	7(8)	-20(7)	-23(7)
C54	41(7)	90(9)	99(9)	4(8)	-16(7)	-27(7)
C55	45(7)	85(9)	102(9)	5(8)	-23(7)	-24(7)
C56	42(7)	86(9)	95(9)	7(8)	-27(7)	-27(7)
C57	43(7)	93(9)	92(9)	12(8)	-26(7)	-25(7)
C58	47(9)	82(10)	104(11)	2(9)	-23(9)	-21(8)
O61	85(9)	116(9)	96(9)	12(8)	5(8)	23(8)
O62	81(8)	106(9)	93(9)	18(8)	4(8)	23(8)
C61	85(6)	103(7)	93(7)	10(5)	4(5)	15(5)
C62	81(7)	98(7)	92(8)	11(7)	3(7)	20(6)
C63	80(9)	100(9)	95(9)	13(8)	-1(8)	23(8)
C64	81(9)	96(9)	97(10)	14(8)	-2(8)	30(8)
C65	82(9)	95(9)	100(10)	14(8)	0(8)	27(8)
C66	82(9)	97(9)	97(9)	12(8)	3(8)	22(8)
C67	82(9)	96(9)	95(9)	11(8)	4(8)	22(8)
C68	85(11)	95(11)	105(11)	14(10)	-2(10)	29(10)
O71	50(7)	72(7)	74(7)	-15(7)	-20(6)	-18(6)

O72	48(7)	71(7)	72(7)	-10(7)	-9(6)	-12(6)
C71	50(5)	72(5)	70(6)	-8(5)	-14(5)	-13(4)
C72	48(6)	82(7)	78(7)	-10(6)	-27(6)	-15(5)
C73	51(7)	92(8)	86(8)	-13(7)	-31(7)	-19(7)
C74	55(8)	96(8)	93(8)	-9(8)	-32(7)	-19(7)
C75	53(7)	95(8)	96(8)	-9(7)	-34(7)	-23(7)
C76	52(8)	92(8)	93(8)	-7(8)	-29(7)	-20(7)
C77	48(7)	87(8)	87(8)	-7(7)	-31(7)	-18(6)
C78	54(9)	98(10)	102(10)	-10(9)	-34(9)	-24(8)
O81	68(8)	103(8)	76(8)	-26(7)	16(7)	24(7)
O82	81(8)	114(9)	89(9)	-21(8)	2(8)	26(7)
C81	76(6)	103(6)	86(6)	-15(5)	10(5)	20(5)
C82	74(7)	111(8)	100(8)	-11(7)	17(7)	28(7)
C83	75(9)	117(9)	112(9)	-7(8)	14(8)	30(8)
C84	77(9)	119(10)	118(10)	-5(9)	11(8)	35(8)
C85	79(9)	121(10)	117(10)	-5(9)	14(8)	38(8)
C86	78(9)	118(10)	112(10)	-6(9)	22(8)	33(8)
C87	76(9)	113(9)	106(9)	-8(8)	22(8)	30(8)
C88	85(11)	125(12)	122(12)	-4(11)	13(10)	40(10)

Table S12. Bond Lengths for TmSDC.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Tm1	O1	2.53(4)	O42	C41	1.241(7)
Tm1	O12	2.130(15)	C41	C42	1.513(11)
Tm1	O22	2.290(12)	C42	C43	1.364(9)
Tm1	O31	2.278(13)	C42	C47	1.366(9)
Tm1	O41	2.311(13)	C43	C44	1.421(9)
Tm1	O72[1]	2.243(13)	C44	C45	1.346(9)
Tm1	O82[1]	2.258(17)	C45	C46	1.346(9)
Tm2	O2	2.287(17)	C45	C48	1.503(12)
Tm2	O3	2.33(2)	C46	C47	1.422(9)
Tm2	O4	2.37(2)	C48	C68[4]	1.24(2)
Tm2	O11	2.114(15)	O51	C51	1.239(7)
Tm2	O21	2.289(13)	O52	C51	1.239(7)
Tm2	O51	2.202(12)	C51	C52	1.510(11)
Tm2	O61	2.184(15)	C52	C53	1.366(9)
Tm3	O5	2.35(3)	C52	C57	1.364(9)
Tm3	O32[2]	2.400(16)	C53	C54	1.422(9)
Tm3	O42[2]	2.268(18)	C54	C55	1.346(9)
Tm3	O52	2.333(14)	C55	C56	1.346(9)
Tm3	O62	2.130(16)	C55	C58	1.501(12)
Tm3	O71	2.314(12)	C56	C57	1.419(9)
Tm3	O81	2.155(14)	C58	C78[6]	1.23(2)

O11	C11	1.241(7)	O61	C61	1.238(7)
O12	C11	1.239(7)	O62	C61	1.240(7)
C11	C12	1.512(11)	C61	C62	1.511(11)
C12	C13	1.366(9)	C62	C63	1.365(9)
C12	C17	1.364(9)	C62	C67	1.365(9)
C13	C14	1.422(9)	C63	C64	1.420(9)
C14	C15	1.346(9)	C64	C65	1.346(9)
C15	C16	1.345(9)	C65	C66	1.346(9)
C15	C18	1.501(12)	C65	C68	1.503(12)
C16	C17	1.421(9)	C66	C67	1.421(9)
C18	C38^{3}	1.24(2)	C68	C48^{7}	1.24(2)
O21	C21	1.242(7)	O71	C71	1.241(7)
O22	C21	1.241(7)	O72	Tm1^{2}	2.244(13)
C21	C22	1.514(11)	O72	C71	1.241(7)
C22	C23	1.368(9)	C71	C72	1.512(10)
C22	C27	1.365(9)	C72	C73	1.365(9)
C23	C24	1.421(9)	C72	C77	1.364(9)
C24	C25	1.346(9)	C73	C74	1.421(9)
C25	C26	1.346(9)	C74	C75	1.344(9)
C25	C28	1.502(12)	C75	C76	1.344(9)
C26	C27	1.422(9)	C75	C78	1.502(12)
C28	C88^{4}	1.21(2)	C76	C77	1.420(9)
O31	C31	1.240(7)	C78	C58^{8}	1.23(2)
O32	Tm3^{1}	2.400(16)	O81	C81	1.242(7)

O32	C31	1.242(7)	O82	Tm1[2]	2.258(17)
C31	C32	1.512(11)	O82	C81	1.241(7)
C32	C33	1.367(9)	C81	C82	1.514(11)
C32	C37	1.365(9)	C82	C83	1.365(9)
C33	C34	1.423(9)	C82	C87	1.365(9)
C34	C35	1.345(9)	C83	C84	1.420(9)
C35	C36	1.346(9)	C84	C85	1.345(9)
C35	C38	1.502(12)	C85	C86	1.345(9)
C36	C37	1.422(9)	C85	C88	1.502(12)
C38	C18[5]	1.24(2)	C86	C87	1.422(9)
O41	C41	1.240(7)	C88	C28[7]	1.21(2)
O42	Tm3[1]	2.268(18)			

[1]+X,1-Y,-1/2+Z; [2]+X,1-Y,1/2+Z; [3]-1/2+X,1/2+Y,+Z; [4]1/2+X,3/2-Y,-1/2+Z; [5]1/2+X,-1/2+Y,+Z; [6]1/2+X,1/2+Y,+Z; [7]-1/2+X,3/2-Y,1/2+Z; [8]-1/2+X,-1/2+Y,+Z

Table S13. Bond Angles for TmSDC.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O12	Tm1	O1	81.3(8)	C31	O32	Tm3[1]	124.5(11)
O12	Tm1	O22	85.9(6)	O31	C31	O32	126.0(16)
O12	Tm1	O31	128.1(6)	O31	C31	C32	117.7(13)
O12	Tm1	O41	160.3(5)	O32	C31	C32	116.3(14)
O12	Tm1	O72[1]	92.8(6)	C33	C32	C31	120.3(14)
O12	Tm1	O82[1]	77.4(6)	C37	C32	C31	119.6(14)
O22	Tm1	O1	77.0(8)	C37	C32	C33	120.1(15)
O22	Tm1	O41	93.6(6)	C32	C33	C34	117.9(17)
O31	Tm1	O1	136.3(10)	C35	C34	C33	121.9(18)
O31	Tm1	O22	74.5(6)	C34	C35	C36	120.3(17)
O31	Tm1	O41	70.2(6)	C34	C35	C38	120.5(16)
O41	Tm1	O1	79.4(8)	C36	C35	C38	119.2(17)
O72[1]	Tm1	O1	76.4(8)	C35	C36	C37	119.1(17)
O72[1]	Tm1	O22	153.2(5)	C32	C37	C36	120.7(17)
O72[1]	Tm1	O31	125.0(6)	C18[5]	C38	C35	125(2)
O72[1]	Tm1	O41	78.9(5)	C41	O41	Tm1	160.9(13)
O72[1]	Tm1	O82[1]	85.6(6)	C41	O42	Tm3[1]	119.3(13)
O82[1]	Tm1	O1	151.3(10)	O41	C41	O42	130.5(16)
O82[1]	Tm1	O22	119.9(5)	O41	C41	C42	114.1(13)
O82[1]	Tm1	O31	72.3(6)	O42	C41	C42	115.4(14)
O82[1]	Tm1	O41	119.2(6)	C43	C42	C41	123.2(15)

O2	Tm2	O3	147.8(8)	C43	C42	C47	115.6(16)
O2	Tm2	O4	149.3(8)	C47	C42	C41	121.2(15)
O2	Tm2	O21	87.0(5)	C42	C43	C44	121.1(18)
O3	Tm2	O4	62.7(9)	C45	C44	C43	122.0(19)
O11	Tm2	O2	81.7(5)	C44	C45	C48	118.0(17)
O11	Tm2	O3	98.7(6)	C46	C45	C44	118.2(18)
O11	Tm2	O4	99.0(7)	C46	C45	C48	123.8(18)
O11	Tm2	O21	91.2(6)	C45	C46	C47	119.8(19)
O11	Tm2	O51	162.8(6)	C42	C47	C46	123.2(18)
O11	Tm2	O61	86.1(7)	C68[4]	C48	C45	116(2)
O21	Tm2	O3	60.9(7)	C51	O51	Tm2	152.5(14)
O21	Tm2	O4	123.6(7)	C51	O52	Tm3	148.0(8)
O51	Tm2	O2	81.2(5)	O51	C51	C52	113.3(12)
O51	Tm2	O3	96.8(7)	O52	C51	O51	124.5(15)
O51	Tm2	O4	94.7(6)	O52	C51	C52	122.2(13)
O51	Tm2	O21	89.8(6)	C53	C52	C51	122.2(13)
O61	Tm2	O2	89.3(5)	C57	C52	C51	118.3(13)
O61	Tm2	O3	122.9(7)	C57	C52	C53	119.5(14)
O61	Tm2	O4	60.4(7)	C52	C53	C54	121.8(16)
O61	Tm2	O21	175.7(6)	C55	C54	C53	117.1(16)
O61	Tm2	O51	91.7(6)	C54	C55	C56	122.6(16)
O5	Tm3	O32[2]	65.0(8)	C54	C55	C58	120.3(16)
O42[2]	Tm3	O5	125.1(11)	C56	C55	C58	117.0(15)
O42[2]	Tm3	O32[2]	86.3(6)	C55	C56	C57	120.2(16)

O42[2]	Tm3	O52	57.5(6)	C52	C57	C56	118.8(16)
O42[2]	Tm3	O71	80.3(6)	C78[6]	C58	C55	136(2)
O52	Tm3	O5	78.4(9)	C61	O61	Tm2	161.8(16)
O52	Tm3	O32[2]	94.8(6)	C61	O62	Tm3	156.8(14)
O62	Tm3	O5	74.0(9)	O61	C61	O62	126.4(18)
O62	Tm3	O32[2]	137.5(6)	O61	C61	C62	115.8(14)
O62	Tm3	O42[2]	128.3(7)	O62	C61	C62	117.8(15)
O62	Tm3	O52	87.3(7)	C63	C62	C61	118.9(15)
O62	Tm3	O71	83.0(6)	C67	C62	C61	121.9(15)
O62	Tm3	O81	88.9(8)	C67	C62	C63	119.2(16)
O71	Tm3	O5	153.1(10)	C62	C63	C64	119.8(18)
O71	Tm3	O32[2]	132.3(5)	C65	C64	C63	119.8(18)
O71	Tm3	O52	114.7(5)	C64	C65	C66	121.6(18)
O81	Tm3	O5	84.7(9)	C64	C65	C68	115.3(16)
O81	Tm3	O32[2]	77.1(6)	C66	C65	C68	123.1(18)
O81	Tm3	O42[2]	135.2(6)	C65	C66	C67	118.8(19)
O81	Tm3	O52	163.1(5)	C62	C67	C66	120.8(18)
O81	Tm3	O71	81.1(6)	C48[7]	C68	C65	119(2)
C11	O11	Tm2	148.9(15)	C71	O71	Tm3	139.3(10)
C11	O12	Tm1	171.7(8)	C71	O72	Tm1[2]	135.1(11)
O11	C11	C12	117.8(14)	O71	C71	C72	113.7(12)
O12	C11	O11	120.9(16)	O72	C71	O71	130.3(14)
O12	C11	C12	121.3(14)	O72	C71	C72	115.9(12)
C13	C12	C11	123.1(14)	C73	C72	C71	119.9(12)

C17	C12	C11	120.0(14)	C77	C72	C71	118.5(12)
C17	C12	C13	116.9(16)	C77	C72	C73	121.6(14)
C12	C13	C14	121.2(17)	C72	C73	C74	119.1(16)
C15	C14	C13	120.5(18)	C75	C74	C73	119.9(17)
C14	C15	C18	116.1(16)	C74	C75	C78	117.1(15)
C16	C15	C14	119.6(17)	C76	C75	C74	120.3(16)
C16	C15	C18	124.3(16)	C76	C75	C78	122.5(17)
C15	C16	C17	120.0(18)	C75	C76	C77	121.8(17)
C12	C17	C16	121.8(17)	C72	C77	C76	117.3(15)
C38[3]	C18	C15	132(2)	C58[8]	C78	C75	128(2)
C21	O21	Tm2	141.9(10)	C81	O81	Tm3	149.8(14)
C21	O22	Tm1	137.7(9)	C81	O82	Tm1[2]	130.1(14)
O21	C21	C22	112.3(12)	O81	C81	C82	115.5(13)
O22	C21	O21	131.2(15)	O82	C81	O81	131.0(16)
O22	C21	C22	116.5(12)	O82	C81	C82	113.4(14)
C23	C22	C21	121.0(13)	C83	C82	C81	117.6(15)
C27	C22	C21	120.5(13)	C83	C82	C87	118.5(16)
C27	C22	C23	118.5(15)	C87	C82	C81	123.9(15)
C22	C23	C24	120.4(16)	C82	C83	C84	118.5(18)
C25	C24	C23	119.2(16)	C85	C84	C83	123.1(19)
C24	C25	C28	116.8(15)	C84	C85	C88	115.7(17)
C26	C25	C24	122.2(16)	C86	C85	C84	118.4(18)
C26	C25	C28	121.0(16)	C86	C85	C88	125.9(19)
C25	C26	C27	118.3(16)	C85	C86	C87	119.9(19)

C22	C27	C26	121.3(16)	C82	C87	C86	121.6(18)
C88[4]	C28	C25	135(2)	C28[7]	C88	C85	127(2)
C31	O31	Tm1	154.8(13)				

[1]+X,1-Y,-1/2+Z; [2]+X,1-Y,1/2+Z; [3]-1/2+X,1/2+Y,+Z; [4]1/2+X,3/2-Y,-1/2+Z; [5]1/2+X,-1/2+Y,+Z; [6]1/2+X,1/2+Y,+Z; [7]-1/2+X,3/2-Y,1/2+Z; [8]-1/2+X,-1/2+Y,+Z

Table S14. Torsion Angles for TmSDC.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
Tm1	O22	C21	O21	53.6(14)	O41	C41	C42	C47	180.0(5)
Tm1	O22	C21	C22	-126.4(15)	O42	C41	C42	C43	-180.0(5)
Tm1	O31	C31	O32	-39(3)	O42	C41	C42	C47	-0.1(6)
Tm1	O31	C31	C32	141(3)	C41	C42	C43	C44	179.8(5)
Tm1	O41	C41	O42	23(3)	C41	C42	C47	C46	-179.8(5)
Tm1	O41	C41	C42	-157(3)	C42	C43	C44	C45	-0.1(10)
Tm1[1]	O72	C71	O71	20.3(10)	C43	C42	C47	C46	0.1(9)
Tm1[1]	O72	C71	C72	-159.7(10)	C43	C44	C45	C46	0.0(9)
Tm1[1]	O82	C81	O81	-20.0(10)	C43	C44	C45	C48	-180.0(6)
Tm1[1]	O82	C81	C82	160.2(11)	C44	C45	C46	C47	0.1(9)
Tm2	O11	C11	O12	7.6(13)	C44	C45	C48	C68[4]	167(2)
Tm2	O11	C11	C12	-172.4(13)	C45	C46	C47	C42	-0.1(10)
Tm2	O21	C21	O22	42.3(14)	C46	C45	C48	C68[4]	-13(2)
Tm2	O21	C21	C22	-137.6(15)	C47	C42	C43	C44	0.0(9)
Tm2	O51	C51	O52	14.3(17)	C48	C45	C46	C47	-179.9(6)
Tm2	O51	C51	C52	-165.7(18)	O51	C51	C52	C53	0.1(6)
Tm2	O61	C61	O62	0(3)	O51	C51	C52	C57	180.0(4)
Tm2	O61	C61	C62	-180(3)	O52	C51	C52	C53	-179.9(4)
Tm3[2]	O32	C31	O31	30.7(10)	O52	C51	C52	C57	0.0(6)
Tm3[2]	O32	C31	C32	-149.3(10)	C51	C52	C53	C54	-179.8(5)
Tm3[2]	O42	C41	O41	-12.2(7)	C51	C52	C57	C56	179.9(4)

Tm3[2]	O42	C41	C42	167.9(8)	C52	C53	C54	C55	-0.4(9)
Tm3	O52	C51	O51	-83(2)	C53	C52	C57	C56	-0.1(8)
Tm3	O52	C51	C52	97(2)	C53	C54	C55	C56	0.4(9)
Tm3	O62	C61	O61	47(3)	C53	C54	C55	C58	-179.8(5)
Tm3	O62	C61	C62	-133(3)	C54	C55	C56	C57	-0.3(9)
Tm3	O71	C71	O72	-39.5(12)	C54	C55	C58	C78[6]	-32(3)
Tm3	O71	C71	C72	140.5(12)	C55	C56	C57	C52	0.2(9)
Tm3	O81	C81	O82	8.5(18)	C56	C55	C58	C78[6]	148(3)
Tm3	O81	C81	C82	-171.7(18)	C57	C52	C53	C54	0.3(9)
O11	C11	C12	C13	0.1(6)	C58	C55	C56	C57	179.9(5)
O11	C11	C12	C17	179.9(4)	O61	C61	C62	C63	-0.2(6)
O12	C11	C12	C13	-179.9(4)	O61	C61	C62	C67	180.0(4)
O12	C11	C12	C17	-0.1(6)	O62	C61	C62	C63	179.9(4)
C11	C12	C13	C14	-179.9(4)	O62	C61	C62	C67	0.0(6)
C11	C12	C17	C16	179.8(4)	C61	C62	C63	C64	179.9(5)
C12	C13	C14	C15	-0.1(8)	C61	C62	C67	C66	180.0(5)
C13	C12	C17	C16	-0.4(8)	C62	C63	C64	C65	0.3(9)
C13	C14	C15	C16	0.1(8)	C63	C62	C67	C66	0.1(9)
C13	C14	C15	C18	-179.9(5)	C63	C64	C65	C66	-0.2(9)
C14	C15	C16	C17	-0.3(8)	C63	C64	C65	C68	179.8(5)
C14	C15	C18	C38[3]	20(2)	C64	C65	C66	C67	0.1(9)
C15	C16	C17	C12	0.4(8)	C64	C65	C68	C48[7]	168(2)
C16	C15	C18	C38[3]	-160(2)	C65	C66	C67	C62	0.0(9)
C17	C12	C13	C14	0.2(8)	C66	C65	C68	C48[7]	-12(2)

C18	C15	C16	C17	179.7(5)	C67	C62	C63	C64	-0.2(9)
O21	C21	C22	C23	-0.2(6)	C68	C65	C66	C67	-179.9(5)
O21	C21	C22	C27	179.9(5)	O71	C71	C72	C73	0.0(6)
O22	C21	C22	C23	179.9(4)	O71	C71	C72	C77	179.9(4)
O22	C21	C22	C27	0.0(6)	O72	C71	C72	C73	-180.0(4)
C21	C22	C23	C24	-180.0(5)	O72	C71	C72	C77	-0.1(6)
C21	C22	C27	C26	179.7(5)	C71	C72	C73	C74	-179.9(5)
C22	C23	C24	C25	0.3(9)	C71	C72	C77	C76	180.0(5)
C23	C22	C27	C26	-0.2(9)	C72	C73	C74	C75	0.0(9)
C23	C24	C25	C26	-0.2(10)	C73	C72	C77	C76	-0.2(9)
C23	C24	C25	C28	-179.8(5)	C73	C74	C75	C76	-0.3(9)
C24	C25	C26	C27	-0.1(9)	C73	C74	C75	C78	-179.9(5)
C24	C25	C28	C88[4]	-179(2)	C74	C75	C76	C77	0.4(10)
C25	C26	C27	C22	0.3(9)	C74	C75	C78	C58[8]	-147(2)
C26	C25	C28	C88[4]	2(3)	C75	C76	C77	C72	-0.1(9)
C27	C22	C23	C24	-0.1(9)	C76	C75	C78	C58[8]	33(3)
C28	C25	C26	C27	179.5(6)	C77	C72	C73	C74	0.2(9)
O31	C31	C32	C33	-0.2(6)	C78	C75	C76	C77	179.9(6)
O31	C31	C32	C37	179.8(4)	O81	C81	C82	C83	0.1(6)
O32	C31	C32	C33	179.9(4)	O81	C81	C82	C87	179.8(5)
O32	C31	C32	C37	-0.1(6)	O82	C81	C82	C83	-180.0(4)
C31	C32	C33	C34	-179.9(5)	O82	C81	C82	C87	-0.3(7)
C31	C32	C37	C36	179.8(5)	C81	C82	C83	C84	179.8(5)
C32	C33	C34	C35	0.1(9)	C81	C82	C87	C86	-179.7(5)

C33	C32	C37	C36	-0.1(9)	C82	C83	C84	C85	-0.1(10)
C33	C34	C35	C36	-0.1(9)	C83	C82	C87	C86	0.0(9)
C33	C34	C35	C38	-179.9(5)	C83	C84	C85	C86	0.0(10)
C34	C35	C36	C37	0.0(9)	C83	C84	C85	C88	-180.0(6)
C34	C35	C38	C18[5]	-171(2)	C84	C85	C86	C87	0.1(9)
C35	C36	C37	C32	0.1(9)	C84	C85	C88	C28[7]	154(2)
C36	C35	C38	C18[5]	9(2)	C85	C86	C87	C82	-0.1(10)
C37	C32	C33	C34	0.0(9)	C86	C85	C88	C28[7]	-26(3)
C38	C35	C36	C37	179.8(5)	C87	C82	C83	C84	0.1(9)
O41	C41	C42	C43	0.1(6)	C88	C85	C86	C87	-179.9(6)

[1]+X,1-Y,1/2+Z; [2]+X,1-Y,-1/2+Z; [3]-1/2+X,1/2+Y,+Z; [4]1/2+X,3/2-Y,-1/2+Z; [5]1/2+X,-1/2+Y,+Z; [6]1/2+X,1/2+Y,+Z; [7]-1/2+X,3/2-Y,1/2+Z; [8]-1/2+X,-1/2+Y,+Z

Table S15. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for TmSDC.

Atom	*x*	*y*	*z*	U(eq)
H13	3693	7553	2084	97
H14	2969	7870	1854	100
H16	3152	6850	476	101
H17	3876	6535	701	98
H18	2398	7324	767	102
H23	6158	7950	1978	78
H24	6898	8336	1878	80
H26	7049	6615	785	79
H27	6310	6218	889	78
H28	7570	8204	1514	88
H33	6070	4797	1205	104
H34	6756	4354	1523	103
H36	6814	2552	480	104
H37	6128	2972	153	103
H38	7374	3395	1550	104
H43	6090	6947	44	110
H44	6755	7605	-131	113
H46	6909	6247	-1392	114
H47	6242	5588	-1221	113
H48	7392	7933	-669	112

H53	6239	7523	2968	94
H54	6957	7961	3173	92
H56	6934	6483	4410	89
H57	6217	6038	4206	91
H58	7491	7501	4325	93
H63	3848	7611	2971	110
H64	3127	8090	3101	110
H66	3052	6824	4419	110
H67	3773	6336	4293	109
H68	2485	8275	3597	114
H73	4004	4299	3709	92
H74	3334	3791	3380	98
H76	3205	2339	4606	95
H77	3872	2826	4954	88
H78	2778	2698	3375	102
H83	3942	6790	4979	122
H84	3301	7482	5235	126
H86	3253	6214	6540	123
H87	3896	5509	6301	118
H88	2791	7939	5849	133

Experimental

Single crystals of $C_{64}H_{40}O_{21}Tm_3$ **[**TmSDC] **were** crystallised solvothermally. A suitable crystal was selected and mounted on a Saxi-CrysAlisPro-abstract goniometer imported SAXI images diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2 [1], the structure was solved with the XT [2] structure solution program using Intrinsic Phasing and refined with the XL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.

2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.
3. Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

Crystal structure determination of [TmSDC]

Crystal Data for $C_{64}H_{40}O_{21}Tm_3$ (M =1651.75 g/mol): monoclinic, space group Cc (no. 9), a = 30.4920(8) Å, b = 15.9861(7) Å, c = 25.7022(13) Å, β = 89.991(3)°, V = 12528.5(9) Å^3, Z = 4, T = 100(2) K, μ(MoKα) = 2.144 mm^{-1}, *Dcalc* = 0.876 g/cm^3, 34959 reflections measured (4.144° ≤ 2Θ ≤ 50.048°), 19378 unique (R_{int} = 0.0404, R_{sigma} = 0.0541) which were used in all calculations. The final R_1 was 0.0745 (I > 2σ(I)) and wR_2 was 0.2053 (all data).

Refinement model description

Number of restraints - 2125, number of constraints - unknown.

Details:

```
1. Twinned data refinement
 Scales: 0.29(3) 0.203(17) 0.265(19) 0.239(17)
2. Fixed Uiso
 At 1.2 times of:
  All C(H) groups
3. Restrained distances
 Tm3-O5
 2.34 with sigma of 0.05
 Tm1-O1
 2.34 with sigma of 0.05
 Tm2-O3
 2.34 with sigma of 0.02
 Tm2-O4
 2.34 with sigma of 0.02
 O3-O4
 2.5 with sigma of 0.02
 Tm2-O2
 2.34 with sigma of 0.05
 C18-C38_$1 ≈ C28-C88_$2 ≈ C48-C68_$2 ≈ C58-C78_$3
 with sigma of 0.02
 O5-O62 ≈ O5-O32_$4
 with sigma of 0.05
 O5-O52 ≈ O5-O81
 with sigma of 0.05
 O1-O12 ≈ O1-O41
 with sigma of 0.05
 O1-O22 ≈ O1-O72_$5
 with sigma of 0.05
 O3-O21 ≈ O4-O61
 with sigma of 0.02
 O3-O11 ≈ O3-O51 ≈ O4-O11 ≈ O4-O51
 with sigma of 0.02
 O2-O11 ≈ O2-O51
 with sigma of 0.02
 O2-O21 ≈ O2-O61
 with sigma of 0.02
4. Restrained planarity
 O11, O12, C11, C12, C13, C14, C15, C16, C17, C18
 with sigma of 0.005
 O21, O22, C21, C22, C23, C24, C25, C26, C27, C28
 with sigma of 0.005
 O31, O32, C31, C32, C33, C34, C35, C36, C37, C38
 with sigma of 0.005
 O41, O42, C41, C42, C43, C44, C45, C46, C47, C48
 with sigma of 0.005
 O51, O52, C51, C52, C53, C54, C55, C56, C57, C58
 with sigma of 0.005
 O61, O62, C61, C62, C63, C64, C65, C66, C67, C68
```

with sigma of 0.005
O71, O72, C71, C72, C73, C74, C75, C76, C77, C78
with sigma of 0.005
O81, O82, C81, C82, C83, C84, C85, C86, C87, C88
with sigma of 0.005
5. Uiso/Uaniso restraints and constraints
All non-hydrogen atoms have similar U: within 2A with sigma of 0.005 and sigma for terminal atoms of 0.01
Uanis(C11) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(C41) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(C21) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(C31) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(O1) ≈ Ueq: with sigma of 0.004 and sigma for terminal atoms of 0.008
Uanis(O3) ≈ Ueq, Uanis(O4) ≈ Ueq: with sigma of 0.0045 and sigma for terminal atoms of 0.009
Uanis(O2) ≈ Ueq: with sigma of 0.005 and sigma for terminal atoms of 0.01
Uanis(C61) ≈ Ueq, Uanis(C71) ≈ Ueq, Uanis(C81) ≈ Ueq: with sigma of 0.005 and sigma for terminal atoms of 0.01
Uanis(O1) = Uanis(O5)
Uanis(O3) = Uanis(O4)
6. Rigid body (RIGU) restrains
O11, O12, C11, C12, C13, C14, C15, C16, C17, C18
with sigma for 1-2 distances of 0.001 and sigma for 1-3 distances of 0.001
O41, O42, C41, C42, C43, C44, C45, C46, C47, C48
with sigma for 1-2 distances of 0.001 and sigma for 1-3 distances of 0.001
O21, O22, C21, C22, C23, C24, C25, C26, C27, C28
with sigma for 1-2 distances of 0.001 and sigma for 1-3 distances of 0.001
O31, O32, C31, C32, C33, C34, C35, C36, C37, C38
with sigma for 1-2 distances of 0.001 and sigma for 1-3 distances of 0.001
7. Same fragment restrains
{O12, O11, C11, C12, C17, C16, C15, C14, C13, C18} sigma for 1-2: 0.005, 1-3: 0.04
{O21, O22, C21, C22, C23, C24, C25, C26, C27, C28} sigma for 1-2: 0.005, 1-3: 0.04
{O31, O32, C31, C32, C33, C34, C35, C36, C37, C38} sigma for 1-2: 0.005, 1-3: 0.04
{O41, O42, C41, C42, C43, C44, C45, C46, C47, C48} sigma for 1-2: 0.005, 1-3: 0.04
{O51, O52, C51, C52, C53, C54, C55, C56, C57, C58} sigma for 1-2: 0.005, 1-3: 0.04
{O61, O62, C61, C62, C63, C64, C65, C66, C67, C68} sigma for 1-2: 0.005, 1-3: 0.04
{O71, O72, C71, C72, C73, C74, C75, C76, C77, C78} sigma for 1-2: 0.005, 1-3: 0.04
{O81, O82, C81, C82, C83, C84, C85, C86, C87, C88} sigma for 1-2: 0.005, 1-3: 0.04
as
{O11, O12, C11, C12, C13, C14, C15, C16, C17, C18}
8.a Aromatic/amide H refined with riding coordinates:
C13(H13), C14(H14), C16(H16), C17(H17), C18(H18), C23(H23), C24(H24), C26(H26), C27(H27), C28(H28), C33(H33), C34(H34), C36(H36), C37(H37), C38(H38), C43(H43), C44(H44), C46(H46), C47(H47), C48(H48), C53(H53), C54(H54), C56(H56), C57(H57), C58(H58), C63(H63), C64(H64), C66(H66), C67(H67), C68(H68), C73(H73), C74(H74), C76(H76), C77(H77), C78(H78), C83(H83), C84(H84), C86(H86), C87(H87), C88(H88)

This report has been created with Olex2, compiled on 2016.08.25 svn.r3337 for OlexSys. Please let us know if there are any errors or if you would like to have additional features.

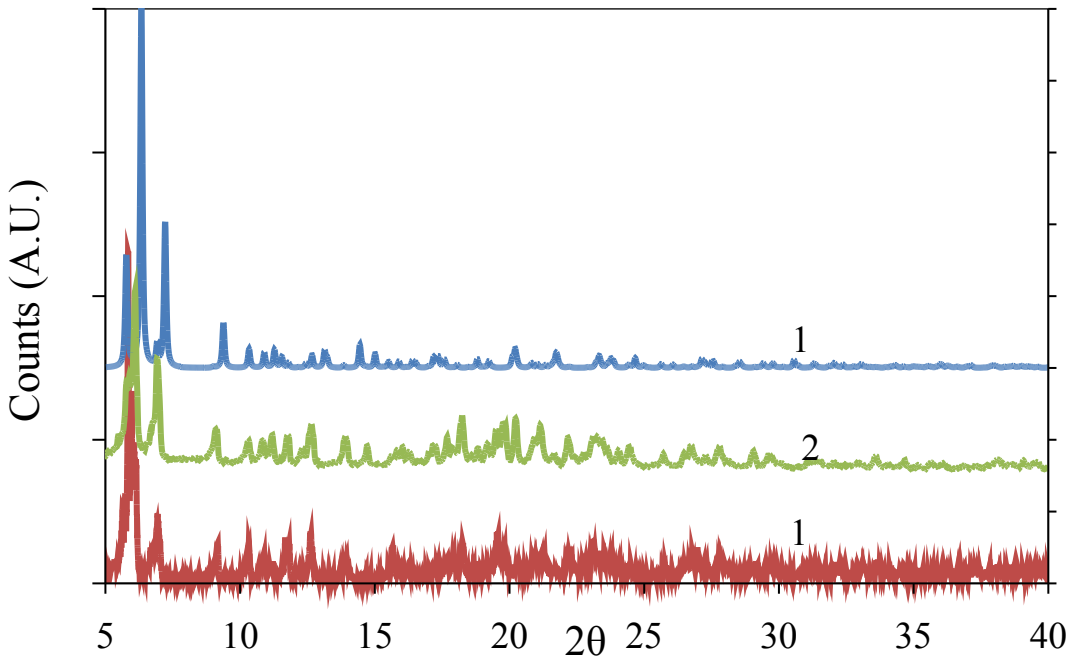

Figure S5. PXRD patterns of **1** and **2** after multiple washes with fresh DEF, and the simulated pattern from single crystal data for **1**.

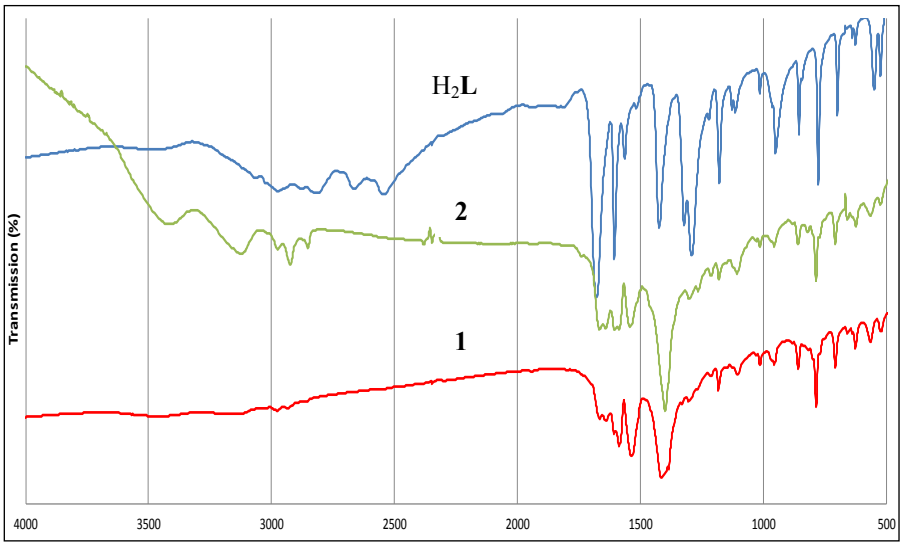

Figure S6. FTIR spectrum of (a) **1**, (b) **2** and (c) H_2**L**.

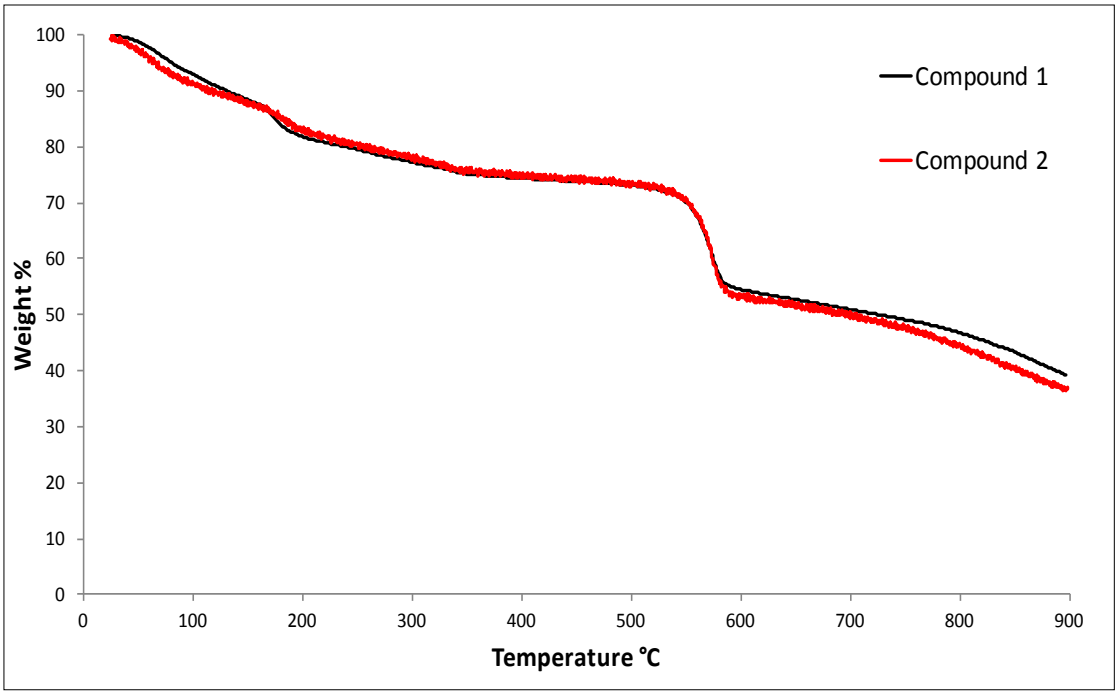

Figure S7. Thermogravimetric curves for **1** and **2**.

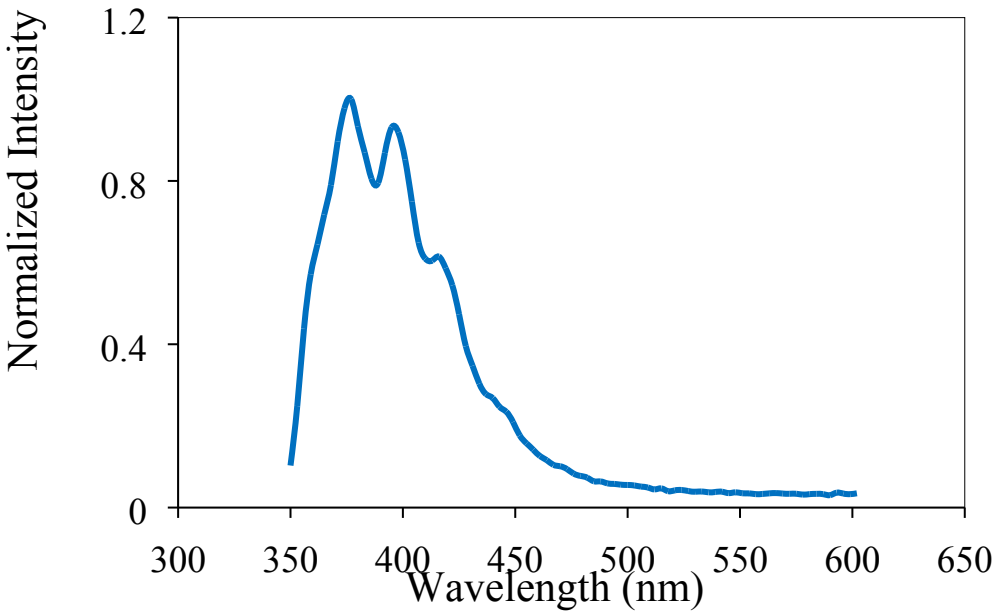

Figure S8. Normalized photoluminescence spectrum of Na_2L solution (Excitation at 341 nm).

Table S16. Photo and radioluminescence decay lifetimes for **2** and H_2**L**.

ID	τ_1 (ns)	α_1%	τ_2 (ns)	α_2%
Photoluminescence*				
H_2L	0.8	74	1.7	26
2	0.4	89	1.7	11
Radioluminescence	$\tau_{s\ prompt}$	α_1%	$\tau_{s\ delayed}$ (ns)	
H_2L	2.0	68	10	-
2	1.2	89	10	-

*Decay curves were fitted by the equation, $I(t) = \alpha_1 \exp\left(-t/\tau_1\right) + \alpha_2 exp(-t/\tau_2)$, where I is the intensity, α is the pre-exponential factor, t is the time, τ_1 and τ_2 are lifetimes. All samples were excited at 341 nm and emission was collected at the third vibronic peak (440 nm for **2** and 460 for H_2**L**)